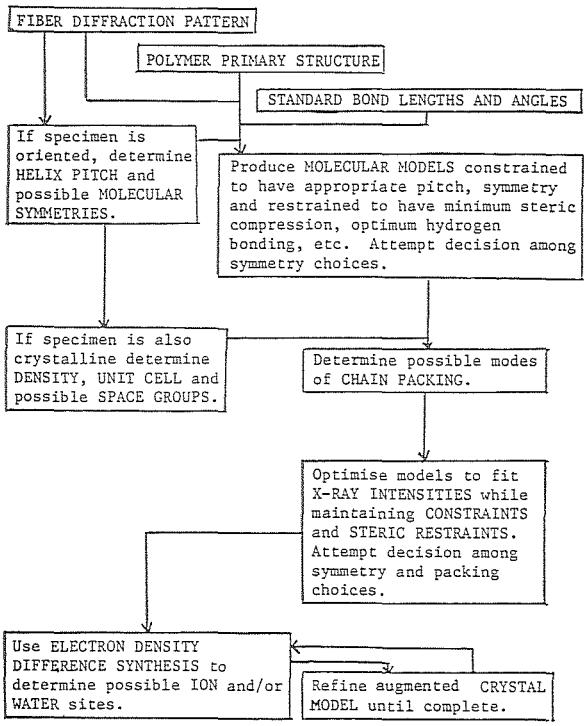
10.X-01 ORDERED STRUCTURES OF POLYPEPTIDES AND PROTEINS. By H. A. Scheraga, Baker Laboratory of Chemistry, Cornell University, Ithaca, N. Y. 14853.

The structures and lattice energies of crystals of small molecules are used to parameterize empirical potential energy functions; the latter are employed in conformational energy calculations on polypeptides and proteins in solution and in the crystalline state. Such calculations provide insights into the types of structures adopted by low-molecular-weight oligopeptides, synthetic polymers and co-polymers of amino acids, and fibrous and globular proteins, in response to intra- and inter-molecular interactions. For example, they can account for structures of open-chain and cyclic oligopeptides, for polymorphism in crystals of polyamino acids (and the temperature-induced interconversion between various crystal forms), for inter-strand complex formation in a fibrous protein such as collagen [using synthetic polytripeptides (containing a glycine residue in each tripeptide unit) as models of collagen], and for the nature of ordered (α and β) structures in globular proteins (i.e. the stabilities of left or right-handed α-helices, and of left- or right-handed β sheets). Each of these examples will be discussed as illustrations of the applicability of conformational energy calculations.

10.X-02 X-RAY DIFFRACTION ANALYSIS OF FIBROUS POLYMERS. By Struther Arnott, Department of Biological Sciences, Purdue University, West Lafayette, IN 47907, U.S.A.



X-ray diffraction can be used to help determine the molecular architecture of the many biologically or industrially important macromolecules (such as DNA, collagen, cellulose, pectin) which are linear polymers that prefer to be long helices rather than more complexly folded structures. It is usually possible to prepare uniaxially oriented specimens in which such helical molecules are aligned with their long axes parallel. Often further lateral organisation occurs but rarely to the degree of a three-dimensionally ordered single crystal. Nevertheless, the modern version (Smith and Arnott, Acta Cryst. (1978), A34, 3-11) of the linked-atom least-squares method (Arnott and Wonacott, Polymer (1966) 7, 157-166) provides a means of augmenting the relatively sparse X-ray data from fibers with non-controversial stereochemical information as outlined in the chart above. The result can be quite detailed, accurate visualisations of (for example) DNA interacting with an intercalating drug (Arnott *et al*, Nature (1980) 287, 561-3) or of specific cations acting as conformational determinants of connective tissue polysaccharide molecules (Cael *et al*, J. Mol. Biol. (1978) 125, 21-42).

10.1-01 CRYSTAL BENDING EFFECTS IN LINEAR POLYMERS. Barbara Moss and Douglas L. Dorset, Medical Foundation of Buffalo, Inc., 73 High St., Buffalo, NY 14203, U.S.A.

Electron diffraction data are usually assigned considerably lower thermal parameters than X-ray data obtained at the same temperature, presumably due to some systematic error in one of the data sets. Using the model proposed by Cowley (Acta Cryst. (1961) 14, 920), crystal bending may be simulated through the smearing-out of Patterson peaks. The diffraction intensities calculated from the Patterson map are then modified through a term somewhat like a temperature factor. The extent of the bend effects depends on the unit cell orientation. Zones where the electron beam is parallel to a long crystallographic axis will exhibit the largest effects. Neglect of bending may be a major cause of the large discrepancies between electron and X-ray temperature factors.

The available experimental electron diffraction data for alpha-poly(3,3-bis(chloromethyl)oxacyclobutane), referred to as BCMO (Claffey *et al*, Phil. Mag. (1974) 30, 1223), nigeran (Pérez *et al*, J. Med. Biol. (1979) 129, 113) and poly(trimethylene terephthalate), denoted TMTP (Poulin-Dandurand *et al*, Polymer (1979) 20, 419) have been re-investigated to determine the extent of bending and dynamical effects. The microcrystals of these materials are characteristically very thin (100Å), and calculations based on the Cowley-Moodie N-beam theory (Acta Cryst. (1957) 10, 609) confirm that dynamical scattering effects are small.

The polymers display varying characteristics. BCMO forms thin (60Å) rigid crystals. No bend contours were observed (Claffey *et al*) and calculations confirm the lack of bending. Allowance for crystal bending of 2° and realistic temperature factors leads to considerably improved agreement between observed and calculated structure factors for nigeran. Similar results are obtained for