TMTP, where bending of 8° is indicated.

Crystal bending may seriously modify electron diffraction data and should be included in the analysis of these materials. This will generally lead to more realistic temperature factors and considerably improved agreement with experiment, facilitating crystal structure determinations.

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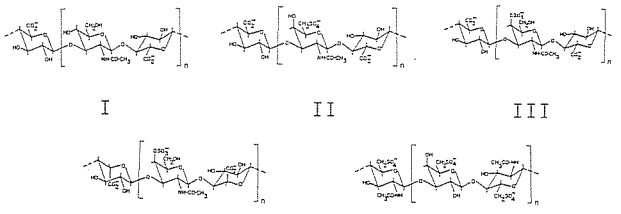
10.3-01 CONNECTIVE TISSUE POLYSACCHARIDES: CATIONS AS DETERMINANTS OF CONFORMATIONS. By Struther Arnott and A. K. Mitra, Department of Biological Sciences, Purdue University, West Lafayette, IN 47907, U.S.A.



I II III

IV V

The glycosaminoglycans, hyaluronate (I), chondroitin 6-sulfate (II) and 4-sulfate (III), dermatan sulfate (IV), keratan sulfate (V), found in connective tissues are linear, polyanionic polydisaccharides in which successive sugar units are linked alternately 1→3 and 1→4 diequatorially. Similar 2_1 helices have been observed for all. Similar 3_2 helices have been trapped for all except (V). 8_3 helices have been found in (II) and (IV). Hyaluronate is unique in having 4_3 allomorphs of two distinctive kinds. Common intra and inter-cellular cations (K^+,H^+,Na^+,Ca^{2+}) influence the polyanion conformation quite specifically. How they do this has been visualized in detailed fiber diffraction studies in which the polyanion conformations and the sites of water molecules and cations have all been defined.

10.3-02 THE UNIT CELL OF THE LOW TEMPERATURE FORM (PHASE II) OF POLYTETRAFLUOROETHYLENE by J. Weeks, E. S. Clark*, and R. K. Eby, National Bureau of Standards, Washington, DC

The crystal structure of Phase II PTFE has been determined from *X*-ray and electron diffraction data. Remarkable electron diffraction patterns giving highly resolved spots to the 26th layer were obtained from fibers of nearly 100% crystallinity. The layer line heights do not correspond to small integers for the layer line numbers. This nonuniformity is interpreted in terms of a regular but incommensurate helical conformation close to the previously assigned 13/6 = 2.1667 CF_2 groups per turn. Refinement of the layer line data gives a conformation of 2.1598 CF_2 groups per turn or a helix of 473/219 conformation. Quantitative evaluation of the lattice parameters as well as intensity estimates were made from *X*-ray diffraction data. The unit cell is triclinic and contains two chain stems of opposite handedness with repeat distance of c = 614.9 A (chain axis). The cross section of the cell is a' = 9.6478 A, b' = 5.6490 Å, γ' = 90°. The calculated density is 2.344 g/cm^3 for a cell containing 2838 atoms. Several trial structures are proposed based on intensity fit of *X*-ray data. Because of the unusual nature of this structure, very similar structures, differing in only small details of packing give radically different cell constants. The problems of unit cell specification and space group determination (P1 or P$\bar{1}$) will be presented in the poster session.
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10.3-03 CORRELATIONS STRUCTURALES ENTRE LES POLY (n-METHYLENE TEREPHTALATES) ET LEURS COMPOSES MODELES, n = 2 à 6. A. Palmer & F. Brisse, Département de Chimie, Université de Montréal, Montréal, H3C 3V1.

Les structures cristallines des poly(n-méthylène téréphtalates), (nGT), ont été généralement établies par analyse conformationnelle. Dans le cas du 3GT on fit aussi usage de composés modèles apparentés. Afin de confirmer la relation entre la conformation de la partie méthylénique de ces polyesters et celle de la séquence correspondante dans les composés modèles, nous avons synthétisé et déterminé les structures cristallines du dibenzoate de butylène-1,4 (R = 5,4) et du di(*para*-nitrobenzoate) de pentylène-1,5 (R = 6,9) composés apparentés au 4GT et 5GT respectivement. Il existe deux polymorphes du 5GT: une forme α, relâchée et une forme β, tendue. La conformation de la séquence méthylénique du di(*para*nitrobenzoate) de pentylène-1,5 se compare favorablement à celle de la forme β du polyester parent. Contrairement à la molécule étudiée plus haut celle de dibenzoate de butylène-1,4 ne présente aucun élément de symétrie alors que les deux formes (α relâchée et β étirée) du 4GT possèdent un centre de symétrie au milieu de la séquence méthylénique. Toutefois il est possible de considérer deux régions distinctes dans la molécule de dibenzoate de butylène-1,4. L'une d'entre elle s'apparente à la forme α 4GT et l'autre à la forme β 4GT. La comparaison systématique des conformations de polyesters du type nGT avec celles des composés modèles apparentés sera présentée pour n = 2 à 6.