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 = 2.1598 CF groups per turn. Refinement of the layer line data gives a conformation of 2.1598 CF, 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 Å (chain axis). The cross section of the cell is a' = 9.6478 Å, b' = 5.6490 Å, γ' = 90°. The calculated density is 2.366 g/cm³ 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 P1) will be presented in the poster session.

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### 10.3-02 THE UNIT CELL OF THE LOW TEMPERATURE FORM (PHASE III) OF POLYTETRAFLUOROETHYLENE

by J. Weeks, E. S. Clarke*, 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 = 2.1598 CF groups per turn. Refinement of the layer line data gives a conformation of 2.1598 CF, 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 Å (chain axis). The cross section of the cell is a' = 9.6478 Å, b' = 5.6490 Å, γ' = 90°. The calculated density is 2.366 g/cm³ 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 P1) will be presented in the poster session.

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