has lattice constants a = 13.8 Å (fiber axis), b = 32.4, c = 9.25 Å. The true primitive monoclinic cell has axes a = 17.6, b = 9.25, c = 13.8 Å, β = 113°. The relation between the two cells is shown in Fig. 1. The mmm symmetry is caused by pseudoorthorhombic (100) or (010) twinning of enantiomorphs.

The nature of the structure causes the absence of large classes of reflections, which are not space group absences. On the pseudo-orthorhombic basis, reflections with h = 0,3,6,8,9, ℓ odd and h = 1,2,4, 7,10, ℓ even were absent. Also no reflection h00 was observed to h = 20. In the CuKα sphere of reflection a total of 429 reflections was observed.

We built a model based on our lattice constants and having three-dimensional order but otherwise having an arrangement similar to that proposed by Prins and Tuinstra.[10] The model incorporated the prior proposal of Prins et al[7] that the sulfur helix has a 13.8 Å period containing ten atoms in three turns of the helix. The model showed that, at least ideally, the space group of the fibrous modification is P2. The arrangement takes advantage of the twofold axes of the $^{10}S_3$ helices; twofold axes, intersecting the helix at right angles, pass through the center of each atom and through points halfway between each pair of atoms (see Fig. 2).

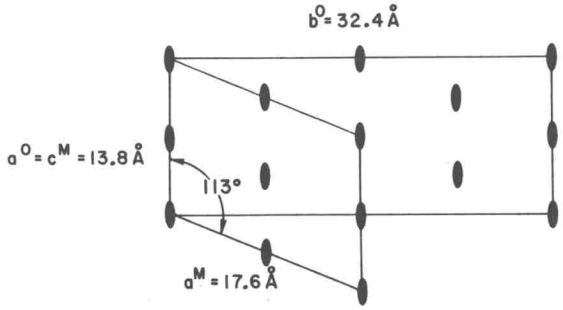

Fig. 1. Relationship between primitive monoclinic (M) and C-face centered orthorhombic (O) unit cells.

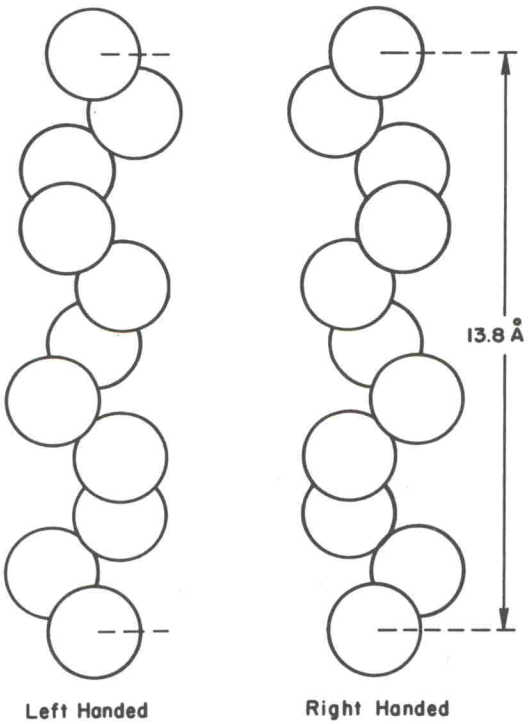

Fig. 2. Idealized sulfur helices.

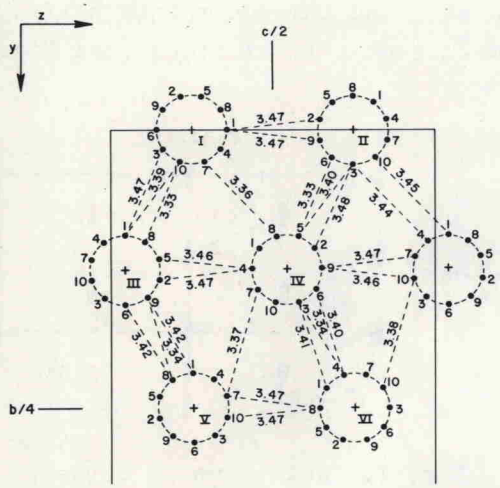

Fig. 3. Projection of the sulfur (II) structure along the fiber axis.

The arrangement is illustrated in Fig. 3. A description based on the pseudo-orthorhombic C-face centered unit cell rather than the primitive cell was used in the structure analysis to facilitate treatment of the twinning. In this description the coordination of the equivalent positions of space group P2 are x, y, z; $\bar{x}$, $\bar{y}$, z; $\frac{1}{2}$ + x, $\frac{1}{2}$ + y,z; and $\frac{1}{2}$ - x, $\frac{1}{2}$ - y,z. These may be used to derive the remainder of the unit cell not shown in Fig. 3. In the figure, the numbering of the atoms in each helix begins with the atom nearest to x = 0. The rows of helices parallel to c have the same hand but in successive rows in the b direction, the hand alternates. Helices I, II, V, and VI are shown as right-handed and helices III and IV as left-handed; these are reversed in the enantiomorph. Eight of the 160 sulfur atoms per unit cell are on twofold axes; these are atoms 1 and 6 of helix I, atoms 3 and 8 of helix VI, and their four equivalents. The remainder of the atoms are in general positions. There are 42 atoms in the asymmetric unit. The structure has 117 independently variable positional parameters and 244 independently variable anisotropic thermal parameters.

Needless to say the total number of observable data, 429, was inadequate for refinement of the total number of parameters, 361 (excluding scale factors). The number of positional parameters was decreased to twelve by assuming the sulfur molecules to be ideal $^{10}S_3$ helices. An overall isotropic temperature factor and a scale factor were adjusted separately. Attempts at refinement of the twelve positional parameters indicated strong correlations between certain pairs and produced large oscillatory parameter changes.[14] When the correlated parameters were deliberately specialized or coupled, reducing the number of variables to