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

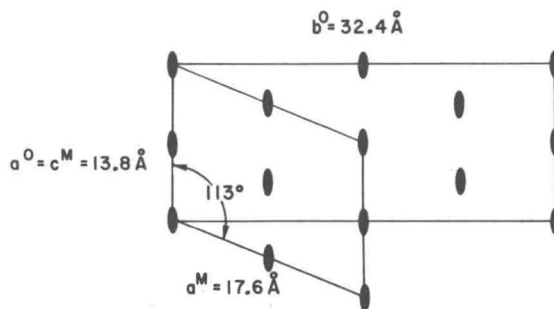each atom and through points halfway between each pair of atoms (see Fig. 2).

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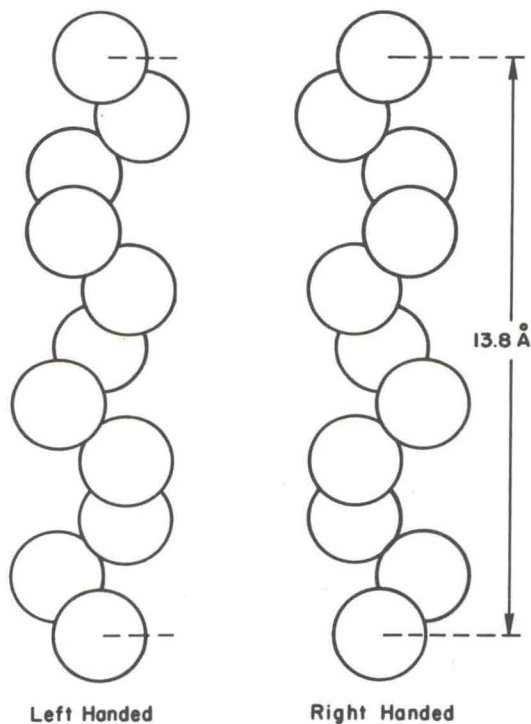

Left Handed   Right Handed
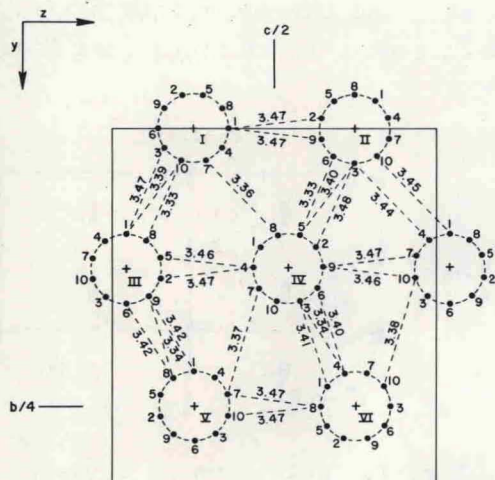
Fig. 2. Idealized sulfur helices.

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 aniso-
tropic 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 deliber-
ately specialized or coupled, re-
ducing the number of variables to