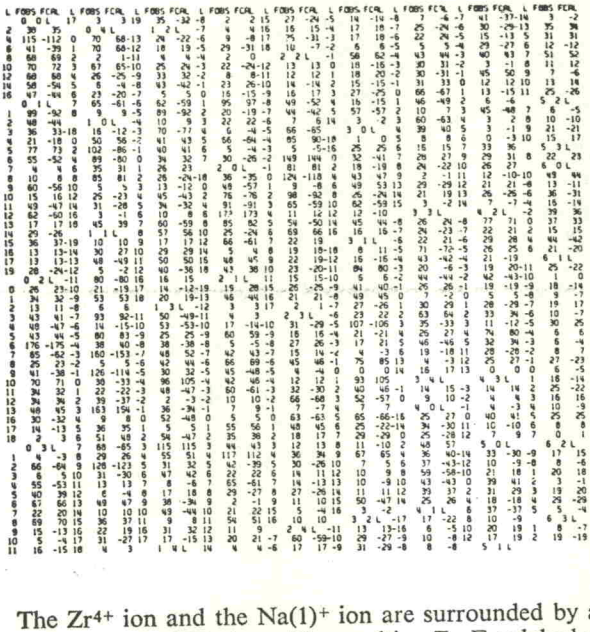
Table 3. *Observed and calculated structure factors for γ-Na_2ZrF_6*



The Zr^{4+} ion and the $Na(1)^+$ ion are surrounded by an irregular array of $7F^-$ ions. The resulting Zr–F polyhedron has nine triangular faces and the Na(1)–F polyhedron has three triangular faces and two trapezium faces. Z... (1948) found similar Zr–7F polyhedra in the st... Na_3ZrF_7. The Zr–F polyhedron shares edges ... Na(1)–F polyhedra and a corner with one other. T... ion is coordinated by $8F^-$ at the corners of an ... trapezohedron. The Zr–F polyhedron shares e... four of the Na(2)–F trapezohedra. There are two ... polyhedra similar to Na(1) and Na(2) with cente... proximately $x=0{\cdot}25$, $y=0{\cdot}04$, $z=0{\cdot}75$ and $x=$ ... $0{\cdot}50$, $z=0{\cdot}90$. These polyhedra are vacant and ... to contain Na or Zr cations. The final difference ... density map has no peaks greater than 1·60 e.Å^{-3} ... tering matter put on the vacant sites does not give ... which converges with a least-squares refinement ... cancies perhaps explain why this polymorph is m... with respect to A-Na_2ZrF_6 below 460°C.

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Indexing of the ψ-sulfur fiber pattern.

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The fiber pattern of ψ-sulfur reported by Tuinstra and the rotation photograph of the pressure-induced fibrous modification of sulfur (II) about the fiber axis (*a*) are essentially the same and have been indexed completely on the pseudo-orthorhombic *C*-face-centered cell with $a=13{\cdot}8$, $b=32{\cdot}4$ and $c=9{\cdot}25$ Å.

We have recently completed a study of the structure of the pressure-induced fibrous form of sulfur (Lind & Geller, 1969). There is strong evidence that this form of sulfur is the same as the ψ-sulfur reported by Prins, Schenk & Wachters (1957; see also Prins & Tuinstra, 1963). Especially important is the exact match of the rotation photograph about the fiber (*a*) axis of a crystal of the pressure-induced phase and that of a fiber pattern of the ψ-sulfur.* Inasmuch as the literature (Tuinstra, 1966, 1967) contains questionable conclusions regarding the indexing of this pattern, it seemed worthwhile to give the results which follow.

It has already been reported (Geller, 1966) that the single-crystal-type diffraction data from the pressure-induced phase indicated that the crystals are *C*-centered orthorhombic with lattice constants $a=13{\cdot}8$, $b=32{\cdot}4$ and $c=9{\cdot}25$ Å. The structure determination (Lind & Geller, 1969) has led to the conclusion that the crystal symmetry is more likely $P2$ and that the apparent orthorhombic symmetry results from a fine-grained twinning. The true monoclinic cell then has the lattice constants $a=17{\cdot}6$, $b=9{\cdot}25$, $c=13{\cdot}8$ Å, $\beta=113°$. The orthorhombic indices listed ... powder pattern (Geller, 1966) may be transform... monoclinic indices by application of the two ... $\frac{1}{2}\bar{1}0|001|100$ and $\frac{1}{2}\frac{1}{2}0|001|\bar{1}00$ to each reflection.

We show the indexing of the rotation phot... Table 1. Listed in the first column are Tuinstra ... observed values, Q_o ($Q=10^4/d^2$), measured on ... photographs of the stretched, CS_2-extracted, ... fibrous sulfur. In the second column, we give ... of Q_o, measured on a rotation photograph (2 hr ... 57·3 mm dia. camera, Cu $K\alpha$ radiation, Ni filter) ... of the same crystal used to obtain the data in ... by Lind & Geller (1969). (The photograph to w... stra (1967) refers is exactly the same except p... exposure time.) We do not list the qualitative i... as we said earlier, the photographs of stretc... extracted, annealed fibrous sulfur and pressur... fibrous sulfur superimpose exactly and quantitati... given in the Lind & Geller (1969) paper. We see ... two sets of Q_o agree quite well although ours are ... ably better resolved. Our Q_c and indices base... pseudo-orthorhombic lattice constants are give... third and fourth columns, respectively. It is see... agreement in Q's is excellent, so that even though ... sible that the fiber axis is very long, as Tuinstra ...

* The best ψ-sulfur photograph we have seen has been made by J. Donohue and S. H. Goodman. This is the one that superposes exactly on our (pseudo-orthorhombic) *a*-axis rotation photograph.