Table I

X-Ray Powder Diffraction Pattern of Tetragonal SnP ($a$ = 3.831 ± 0.001 Å, $c$ = 5.963 ± 0.001 Å)

| I/Io* | h | k | l | d (obs.) | d (calc.) |
|---|---|---|---|---|---|
| 90 | 1 | 0 | 1 | 3.2189 | 3.2226 |
| 100 | 0 | 0 | 2 | 2.9784 | 2.9810 |
| 90 | 1 | 1 | 0 | 2.7105 | 2.7084 |
| 90 | 1 | 1 | 2 | 2.0030 | 2.0046 |
| 80 | 2 | 0 | 0 | 1.9151 | 1.9152 |
| 70 | 1 | 0 | 3 | 1.7625 | 1.7642 |
| 80 | 2 | 1 | 1 | 1.6458 | 1.6464 |
| 70 | 2 | 0 | 2 | 1.6103 | 1.6113 |
| 20 | 0 | 0 | 4 | 1.4901 | 1.4905 |
| 30 | 2 | 2 | 0 | 1.3545 | 1.3542 |
| 30 | 1 | 1 | 4 | 1.3068 | 1.3056 |
| 30 | 2 | 1 | 3 | 1.2972 | 1.2975 |
| 10 | 3 | 0 | 1 | 1.2473 | 1.2485 |
| 30 | 2 | 2 | 2 | 1.2332 | 1.2310 |
| 40 | 3 | 1 | 0 | 1.2111 | 1.2113 |
| 20 | 2 | 0 | 4 | 1.1756 | 1.1762 |
| 10 | 1 | 0 | 5 | 1.1381 | 1.1385 |
| 40 | 3 | 1 | 2 | 1.1224 | 1.1221 |
| 10 | 3 | 0 | 3 | 1.0744 | 1.0742 |
| 10 | 3 | 2 | 1 | 1.0462 | 1.0459 |
| 10 | 2 | 2 | 4 | 1.0018 | 1.0023 |
| 20 | 2 | 1 | 5 | .9784 | .9786 |
| 10 | 4 | 0 | 0 | .9577 | .9576 |
| 10 | 3 | 1 | 4 | .9408 | .9403 |
| 10 | 3 | 2 | 3 | .9370 | .9369 |
| 5 | 4 | 1 | 1 | .9186 | .9179 |
| 10 | 4 | 0 | 2 | .9123 | .9117 |
| 10 | 3 | 3 | 0 | .9026 | .9026 |
| 2 | 2 | 0 | 6 | .8818 | .8820 |
| 5 | 3 | 0 | 5 | .8715 | .8714 |
| 10 | 3 | 3 | 2 | .8645 | .8643 |
| 10 | 4 | 2 | 0 | .8569 | .8565 |
| 10 | 4 | 1 | 3 | .8422 | .8416 |
| 10 | 1 | 0 | 7 | .8318 | .8314 |
| 10 | 4 | 2 | 2 | .8231 | .8232 |
| 5 | 3 | 2 | 5 | .7930 | .7932 |

*Read using the David Mann Film Reader.

Table II

$I_o$ and $I_c$ for Tetragonal SnP

| h | k | l | $I_o$ | $I_c$ |
|---|---|---|---|---|
| 1 | 0 | 1 | | 47.36 |
| −1 | 0 | −1 | | 44.06 |
| | | | 100.00 | 91.43 |
| 0 | 0 | 2 | | 20.93 |
| 0 | 0 | −2 | | 22.13 |
| | | | 36.95 | 43.07 |
| 1 | 1 | 0 | 72.23 | 74.84 |
| 1 | 1 | 2 | | 25.67 |
| −1 | −1 | −2 | | 27.16 |
| | | | 55.41 | 52.83 |
| 2 | 0 | 0 | 26.59 | 25.77 |
| 1 | 0 | 3 | | 13.19 |
| −1 | 0 | −3 | | 11.95 |
| | | | 21.70 | 25.14 |
| 2 | 1 | 1 | | 14.25 |
| −2 | −1 | −1 | | 13.36 |
| | | | 25.70 | 27.61 |
| 2 | 0 | 2 | | 12.41 |
| −2 | 0 | −2 | | 13.16 |
| | | | 27.71 | 25.57 |
| 0 | 0 | 4 | | 1.68 |
| 0 | 0 | −4 | | 1.86 |
| | | | 3.99 | 3.54 |
| 2 | 2 | 0 | 7.60 | 7.76 |
| 1 | 3 | 0 | 12.79 | 10.45 |
| 1 | 2 | 3 | | 9.32 |
| −1 | −2 | −3 | | 8.41 |
| 1 | 1 | 4 | | 4.26 |
| −1 | −1 | −4 | | 4.72 |
| | | | 25.60 | 26.71 |
| 3 | 0 | 1 | | 2.90 |
| −3 | 0 | −1 | | 2.72 |
| | | | 6.50 | 5.61 |
| 2 | 0 | 4 | | 3.01 |
| −2 | 0 | −4 | | 3.34 |
| | | | 6.10 | 6.35 |

No. IDF4, cut out, and weighed. Fourteen pieces of data were collected.

Least-squares refinement based on the function $\Sigma w|I_o - I_c|^2$ was done using a program written by Prewitt[10] which handles the sums of nonequivalent overlapping reflections. Atomic scattering factors[11] corrected for the real and imaginary parts of the anomalous dispersion were used. The imaginary component was applied separately to reflections $hkl$ and $\bar{h}kl$. Occupancy factors were held at 2 and the weighting scheme $w = 1/\sigma^2$, with $\sigma = \sqrt{I_o} + 2.0$, was used. The positions 0, 0, $z$ of space group 14mm were used in the refinement with $z$ held at 0.0 for Sn and $z = 0.4$ initially assumed for P.

One scale factor, the single position parameter for P, and two isotropic temperature factors were varied. The $R$ factor defined as $R = \Sigma|I_o - I_c|/\Sigma I_o$ was reduced to 7.8%. The intensity data and final position parameters are shown in Table II. Bond distances were calculated[12] (Table III). The numbers of the atoms correspond to those in Figure 1.

Table III

Final Parameters and Bond Distances and Angles for Tetragonal SnP

| Atom | Position ($x$, $y$, $z$) | Temp factor, Å² |
|---|---|---|
| Sn | 0, 0, 0 | 0.9 ± 0.3 |
| P | 0, 0, 0.428 ± 0.010 | 2.6 ± 1.6 |

| Atoms[a] | Dist, Å | Atoms | Angles, deg |
|---|---|---|---|
| Sn(1)–P(2) | 2.55 ± 0.06 | P(3)–Sn(1)–P(2) | 99.0 ± 1.2 |
| Sn(1)–P(3) | 2.74 ± 0.01 | P(3)–Sn(1)–P(4) | 81.0 ± 1.2 |
| Sn(1)–P(4) | 3.41 ± 0.06 | P(5)–Sn(1)–P(3) | 88.6 ± 0.4 |

[a] The numbers on the atoms correspond to the numbers of the atoms in Figure 1.

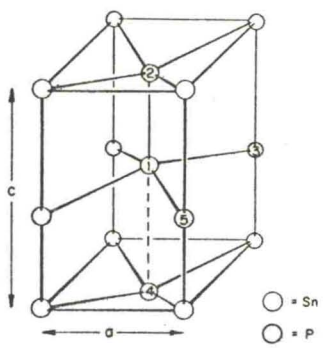


Figure 1.—Structure of SnP.

The cubic structure was shown to be NaCl type. Intensities were read from a Debye–Scherrer pattern using the David Mann film reader. These were compared to the Debye–Scherrer patterns calculated for SnP having the NaCl-type and ZnS-type structures by a program written by Jeitschko and Parthé.[13] The results (Table IV) clearly indicate the NaCl-type structure to be correct. The pattern is similar to that reported by Osugi, *et al.*,[4] to be sphalerite type.

(10) C. T. Prewitt, local unpublished computer program.

(11) "International Tables for X-Ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962, pp 202 and 213, Tables 3.3.1A and 3.3.2A.

(12) L. W. Finger, "University of Minnesota Program for Computing Bond Angles and Distances with Error and Analysis," UMBADTEA, 1965.

(13) W. K. Jeitschko and E. Parthé, unpublished computer program for calculation of X-ray powder diffraction patterns.