*Table 3. Powder pattern for* $In_3Te_4$ (CuK$\alpha$ *radiation*)

| | d (Å) | | Rel. I | | | d (Å) | | Rel. I | |
|---|---|---|---|---|---|---|---|---|---|
| hk·l | obs. | calc. | obs. | calc. | hk·l | obs. | calc. | obs. | calc. |
| 00·3 | 13·5 | 13·53 | VW | 60 | 12·17 | 1·205 | 1·203 | VW | 32 |
| 00·6 | 6·78 | 6·79 | VVW | 20 | 11·30 | 1·142 | 1·142 | VVW | 23 |
| 00·9 | 4·50 | 4·51 | VW | 65 | 02·31 | | 1·068 | | 24 |
| 00·12 | 3·386 | 3·382 | VW | 71 | 22·0 | 1·066 | 1·065 | W–M* | 42 |
| 10·7 | 3·093 | 3·110 | VVS | 1250 | 11·33 | | 1·065 | | 1 |
| 01·8 | 3·006 | 2·992 | VW | 39 | 30·21 | | 1·037 | | 11 |
| 10·10 | 2·729 | 2·732 | W | 76 | 03·21 | 1·039 | 1·037 | VW | 11 |
| 01·14 | 2·272 | 2·278 | M–S | 342 | 22·9 | | 1·036 | | 5 |
| 11·0 | 2·128 | 2·128 | S | 463 | 13·7 | 1·008 | 1·008 | W–M | 65 |
| 11·3 | 2·098 | 2·109 | W | 35 | 11·36 | | 0·9963 | | 18 |
| 10·16 | | 2·097 | | 65 | 30·24 | 0·9955 | 0·9945 | W* | 34 |
| 01·17 | 2·003 | 2·004 | W–M | 97 | 03·24 | | 0·9945 | | 34 |
| 00·21 | 1·934 | 1·932 | W–M | 34 | 31·14 | 0·9648 | 0·9649 | W | 40 |
| 11·9 | | 1·935 | | 37 | 21·31 | 0·9554 | 0·9544 | W | 40 |
| 10·19 | 1·860 | 1·848 | VVW | 15 | 10·43 | | 0·9143 | | 12 |
| 11·12 | 1·800 | 1·801 | VW | 32 | 31·20 | | 0·9136 | | 5 |
| 20·5 | | 1·797 | | 6 | 40·7 | 0·9127 | 0·9109 | VW* | 30 |
| 02·7 | 1·754 | 1·756 | M–S | 215 | 30·30 | | 0·9100 | | 6 |
| 00·24 | 1·691 | 1·691 | VW | 33 | 03·30 | | 0·9100 | | 6 |
| 01·23 | 1·587 | 1·591 | VW | 35 | 00·45 | 0·9021 | 0·9018 | VW* | 3 |
| 20·14 | 1·555 | 1·555 | W–M | 93 | 22·24 | | 0·9011 | | 32 |
| 20·17 | 1·458 | 1·459 | VW | 32 | 04·14 | 0·8785 | 0·8789 | VW* | 19 |
| 11·21 | 1·431 | 1·431 | W | 69 | 12·38 | 0·8491 | 0·8478 | W* | 38 |
| 21·7 | 1·355 | 1·354 | M–S | 166 | 01·47 | | 0·8407 | | 24 |
| 00·30 | | 1·353 | | 5 | 02·43 | | 0·8402 | | 27 |
| 10·28 | | 1·349 | | 10 | 04·20 | 0·8388 | 0·8396 | M* | 3 |
| 12·14 | 1·255 | 1·256 | W–M | 83 | 32·7 | | 0·8375 | | 69 |
| 10·31 | 1·231 | 1·234 | M* | 38 | 22·30 | | 0·8368 | | 14 |
| 00·33 | | 1·230 | | 3 | 23·14 | 0·8130 | 0·8125 | W* | 54 |
| 30·0 | | 1·229 | | 66 | 13·31 | 0·8064 | 0·8062 | M* | 60 |
| 11·27 | | 1·228 | | 8 | 41·0 | | 0·8051 | | 105 |

* Broad line.

the powder photograph. The lattice constants determined from the powder photograph (CuK$\alpha$ radiation) are $a = 4{\cdot}26 \pm 0{\cdot}01$, $c = 40{\cdot}6 \pm 0{\cdot}1$ Å or in the rhombohedral description $\alpha = 13{\cdot}7_5$ Å, $\alpha = 17{\cdot}8_0°$. The powder pattern indexed on the hexagonal basis is given in Table 3. Shown also are qualitatively estimated intensities and those calculated* from

$$I_{rel} = p|F|^2 \times 10^{-5} L{\cdot}P$$

where $p$ is the multiplicity, $F$, the structure factor and $L{\cdot}P$ the Lorentz-polarization factor. The positional parameters were those obtained from the single crystal analysis, and because the program* allows only individual isotropic temperature factors, In(1) and Te(2) were assigned values of 0·5 Å$^2$ and In(2) and Te(1) values of 1·0 Å$^2$.†

When this pressure-induced $In_3Te_4$ phase was heated at 200°C in an evacuated sealed fused silica tube for 67 hr, it decomposed into a mixture of the atmospheric pressure $In_2Te_3$ phase and an NaCl-type phase with composition (determined from the

* The program used was originally derived by TREUTING[20] for the IBM 704 and modified for the IBM 7094 by N. V. Vaughan and A. R. Storm.

† Differences in vibration amplitudes of the atoms were indicated by the results from the single crystal analysis.