

Table 3. Powder pattern for In_3Te_4 ($\text{CuK}\alpha$ radiation)

d (Å)					d (Å)				
		Rel. I					Rel. I		
$h \cdot k \cdot l$	obs.	calc.	obs.	calc.	$h \cdot k \cdot l$	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		1·065	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		1·037	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		0·9945	W*	34
01·17	2·003	2·004	W-M	97	03·24		0·9945		34
00·21		{1·932		{34	31·14	0·9648	0·9649	W	40
11·9	1·934	{1·935	W-M	{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		0·9109	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		0·9018	VW*	3
20·14	1·555	1·555	W-M	93	22·24		0·9011	VW*	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		{1·354		{166	01·47		0·8407		24
00·30	1·355	{1·353	M-S	{5	02·43		0·8402		27
10·28		{1·349		{10	04·20		0·8388	{M*	3
12·14	1·255	1·256	W-M	83	32·7		0·8375		69
10·31		{1·234		{38	22·30		0·8368		14
00·33	1·231	{1·230	M*	{3	23·14	0·8130	0·8125	W*	54
30·0		{1·229		{66	13·31	0·8062	0·8062	M*	60
11·27		{1·228		{8	41·0	0·8064	0·8051		105

* Broad line.

the powder photograph. The lattice constants determined from the powder photograph ($\text{CuK}\alpha$ radiation) are $a = 4·26 \pm 0·01$, $c = 40·6 \pm 0·1$ Å or in the rhombohedral description $\alpha = 13·75$ Å, $\alpha = 17·80^\circ$. The powder pattern indexed on the hexagonal basis is given in Table 3. Shown also are qualitatively estimated intensities and those calculated* from

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

where p is the multiplicity, F , the structure factor

* 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.

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 $0·5$ Å² and In(2) and Te(1) values of $1·0$ Å².†

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

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

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lattice constant appears to f under a pre pressure rele NaCl-type a probable th contains exce

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It appears In_2Te_3 phase known Bi_2Te ably as a sing discern the patterns, be In_3Te_4 -type tures of the t belong to th atoms on th In_3Te_4 has t Te-In-, divi in approxim must have ti dividing the approximatel two phases a one would ex (threefold ax In_3Te_4 is ve constants of

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