

The intensity distribution indicated that all atoms must lie on the threefold axis body diagonal of the rhombohedron (hexagonal *c*-axis) and that ideally, there must be seven atoms in the rhombohedral cell. The ideal formula of the compound appeared to be In_3Te_4 . With this formula the most likely space group to which the crystal belongs is $R\bar{3}m$ with one In(1) in $1a, 000$, the other atoms being in $2c, \pm xxx$ or in the hexagonal description $3a, 000, \pm(\frac{1}{3}\frac{2}{3}\frac{2}{3})$ and $6c, (000, \pm\frac{1}{3}\frac{2}{3}\frac{2}{3}) \pm 00z$. Later it was found that In_3Te_4 has the anti- Sn_4As_3 structure.⁽¹⁰⁾

Table 2. Interatomic distances and standard deviations

Atom	Nearest neighbors	Distance (Å)	σ (Å)
In(1)	6Te(2)	3.02	0.03
In(2)	3Te(1)	2.84	0.03
	3Te(2)	3.24	0.05
Te(1)	3In(2)	2.84	0.03
	3Te(1)	3.98	0.03
Te(2)	3In(1)	3.02	0.03
	3In(2)	3.24	0.05
	Next nearest neighbors		
In(1)	6In(1)	4.27	0.01
	6In(2)	4.57	0.03
In(2)	3In(1)	4.57	0.03
	3Te(1)	5.17	0.05
	6In(2)	4.27	0.01
Te(1)	3In(2)	5.17	0.05
	3Te(2)	4.30	0.03
	6Te(1)	4.27	0.01
Te(2)	3Te(1)	4.30	0.03
	3Te(2)	4.25	0.03
	6Te(2)	4.27	0.01

Intensities of selected reflections from the precession camera photographs were estimated visually by comparison with a calibrated intensity strip. Lorentz-polarization corrections were applied by means of the WASER⁽¹³⁾ and GRENVILLE-WELLS-ABRAHAMS⁽¹⁴⁾ charts. No correction was made for absorption. As in the case of the isostructural Sn_4As_3 , the atoms must be disposed along the hexagonal *c*-axis near multiples of $1/7$. Thus using the relative observed structure amplitudes and the BUEGER tables,⁽¹⁵⁾ adjustments around multiples of $1/7$ were made. The BUSING-MARTIN-LEVY⁽¹⁶⁾ least squares program modified

by Cetlin for the present Bell System IBM 7094 monitor program was then used to refine the parameters. The atomic scattering factors used were from THOMAS and UMEDA,⁽¹⁷⁾ corrected for the real part of the dispersion.⁽¹⁸⁾

The values of the z -parameters obtained were: for In(2), 0.4273; Te(1), 0.1284; and Te(2), 0.2908. Standard errors were 0.0008, 0.0006 and 0.0009 respectively. Except for β_{33} , all other thermal parameters β_{ii} and β_{ij} are zero. β_{33} parameters were also refined, but the standard errors on them indicate that they are essentially indeterminate from the data used. However, because the correlation matrix indicated insignificant interaction⁽¹⁹⁾ with positional parameters, the latter may be considered to be virtually unaffected by the indeterminacy of the thermal parameters.

Interatomic distances and their standard deviations are given in Table 2. In most cases the standard deviations are large. The nearest neighbor coordination of all atoms is octahedral and next nearest neighbor coordination is 12. The In_3Te_4 structure* is related to the NaCl-type structure, but it will be noted (Table 2) that Te(1) has 3In and 3Te (instead of all In) nearest neighbors, In(2) has 9In and 3Te (instead of all Te) and Te(1) has 9Te and 3In (instead of all Te) next nearest neighbors. The In(2)-Te(1) next nearest neighbor distances are rather large because of the large Te(1)-Te(1) contact distances.

The average nearest neighbor In-Te distance is 3.03 ± 0.11 Å. If for the moment, the large limits of error are overlooked, we may compare the average In-Te distance, 3.03 Å with 3.09 Å in the stoichiometric InTe. Because the ratio of trivalent to monovalent In ions in the In_3Te_4 is 5 : 1 as compared with 1 : 1 in InTe, one would expect a substantial decrease in the average size of the In atom; 0.06 Å is substantial, but the large limits of error preclude any assertion regarding the comparison of distances.

FURTHER CHARACTERIZATION OF THE PRESSURE INDUCED In_3Te_4 PHASE

A specimen of In_3Te_4 prepared at ~ 35 kbar and 550°C for 1 hr was very nearly single phase. A slight trace of the NaCl-type phase was seen in

* The reader is referred to Ref. 10 for excellent diagrams of the structure.

Table 3. Powder pattern for In_3Te_4 (CuK α radiation)

$hk\cdot l$	d (Å)		Rel. I		$hk\cdot l$	d (Å)		Rel. I	
	obs.	calc.	obs.	calc.		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				24
00·12	3·386	3·382	VW	71	22·0	1·066	1·068	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		2·109		35	11·36		0·9963		18
10·16	2·098	2·097	W	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		1·932		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		1·801		32	31·20		0·9136		5
20·5	1·800	1·797	VW	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		1·354		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	0·8396	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		1·230		3	23·14	0·8130	0·8125	W*	54
30·0	1·231	1·229	M*	66	13·31		0·8062		60
11·27		1·228		8	41·0	0·8064	0·8051	M*	105

* Broad line.

the powder photograph. The lattice constants determined from the powder photograph (CuK α radiation) are $a = 4.26 \pm 0.01$, $c = 40.6 \pm 0.1$ Å or in the rhombohedral description $\alpha = 13.7_5^\circ$, $\alpha = 17.8_0^\circ$. 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 Å and In(2) and Te(1) values of 1.0 Å.[†]

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.