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 BUERGER 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

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