XRAY system (1976).* Lattice constants were refined from 22 reflections centred on the diffractometer (Ag $K\alpha$ radiation).

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35616 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and interatomic distances* (Å) *for* YNi *up to* 4 Å [*space group Pnma*; *all atoms in* 4(*c*)]

The isotropic temperature factor is expressed as $T = \exp(-2\pi^2 Us^2)$ where $s = 1/d_{hkl}$; U values are Å^2 $\times 10^4$. The values for the isotropic temperature factors are obtained by recalculation from the anisotropic ones. E.s.d.'s are in parentheses and refer to the last significant figure.

	x	y	z	U (Å^2)*
Y	1798 (1)	2500	1325 (2)	92 (2)
Ni	357 (2)	2500	6233 (3)	104 (4)
Y–Ni	2·897 (2)		Ni–Y	2·897 (2)
2Ni	2·898 (1)		2Y	2·898 (1)
2Ni	2·906 (1)		2Y	2·906 (1)
Ni	2·911 (2)		Y	2·911 (2)
Ni	2·991 (2)		Y	2·991 (2)
Y–4Y	3·587 (1)		Ni–2Ni	2·522 (1)
2Y	3·607 (1)		2Ni	3·841 (3)
2Y	3·806 (2)			

* Calculated from $U = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

Discussion. The final atom coordinates and interatomic distances are listed in Table 1. The coordinates agree with those calculated on the basis of ideal stacking which requires that each Y atom should have six equidistant Y neighbours (Klepp & Parthé, 1980).

There is no doubt that YNi crystallizes with the orthorhombic FeB structure. It seems likely that multiple diffraction was the cause of the two weak 0*kl* reflections observed by Smith & Hansen (1965) which led them to assume that YNi has monoclinic symmetry.

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Structure of Copper–Indium Cu_7In_3

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Abstract. Cu_7In_3, triclinic, $P\bar{1}$, $a = 10{\cdot}071\ (5)$, $b = 9{\cdot}126\ (5)$, $c = 6{\cdot}724\ (4)$ Å, $\alpha = 90{\cdot}22\ (3)$, $\beta = 82{\cdot}84\ (3)$, $\gamma = 106{\cdot}81\ (3)°$, $Z = 4$, $V = 586{\cdot}6$ Å^3, $D_c = 8{\cdot}94$, $D_o = 8{\cdot}94$ Mg m^{-3}. $R = 0{\cdot}098$ for 1760 refined reflections. The In atoms are arranged in approximate layers which also contain some of the Cu atoms; the remaining Cu atoms are situated in layers about halfway between these approximate layers.

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Introduction. The cell parameters of the δ phase in the binary system Cu–In have been reported by several authors. Weibke (1939) proposed a cubic cell, Gauneau & Graf (1968) a triclinic one, while according to Fournelle & Clark (1972) the cell is tetragonal with very large parameters. As the structure of this alloy is of interest in understanding alignment in composite materials (Vrolijk & Wolff, 1980) it was desirable to

determine this structure. Vrolijk & Wolff report that the cell is triclinic and that the formula of the δ phase is Cu_7In_3, rather than Cu_9In_4 as is stated, for instance, by Gauneau & Graf.

The method of preparing single crystals is described by Vrolijk & Wolff (1980). A crystal free of twinning was selected by Weissenberg methods, ground to a sphere of radius $r = 0{\cdot}3$ mm and analysed with a computer-controlled PW 1100 four-circle diffractometer using Mo $K\alpha$ radiation filtered with a graphite monochromator. About 3600 reflections were recorded; this yielded a set of 1760 unique reflections, 1719 of which were above the 3σ level. Cell dimensions were obtained by least-squares refinement of the angular positions of 25 reflections. Lorentz–polarization and absorption corrections ($\mu = 36{\cdot}8$ mm^{-1}) were applied.

Intensity statistics indicated that the structure is very probably centrosymmetric, so $P\bar{1}$ was selected as the space group.

The presence of pseudosymmetry in the structure hampered the structure determination. On inspection of a Debye–Scherrer photograph it can easily be seen that there are a limited number of strong lines or line groups. This set is indexable on the basis of a cubic cell with a cell parameter of approximately 9·1 Å (Vrolijk & Wolff, 1980). Furthermore, the reflections with h = odd are generally much weaker than those with h = even. A list with strong reflections contains almost exclusively reflections with h = even, which is unfavourable for the application of direct methods. Yet it was by direct methods, using the *MULTAN* program (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), that the structure was solved. The reflections required in the starting set for phase definition were not generated by the program, but carefully chosen by us. After the crude model had been established, refinement by least-squares methods produced the atomic coordinates and isotropic temperature factors given in Table 1. Because of errors in the intensities due to the high absorption coefficient, refinement was stopped when R was 0·098 ($R = \sum|\Delta F|/\sum|F_o|$ based on all measured reflections).* No attempt was made to refine the temperature factors anisotropically. The In–In and the In(1)–Cu bond lengths are listed in Table 2. Bond lengths of the other In atoms are similar.

Table 1. *Atomic coordinates in the triclinic cell, isotropic temperature factors and standard deviations*

	x	y	z	B (Å^2)
In(1)	0·944 (2)	0·472 (2)	0·793 (2)	0·27 (3)
In(2)	0·634 (2)	0·006 (2)	0·618 (2)	0·30 (3)
In(3)	0·518 (2)	0·720 (2)	0·921 (2)	0·27 (3)
In(4)	0·817 (2)	0·735 (2)	0·142 (2)	0·28 (3)
In(5)	0·104 (2)	0·164 (2)	0·322 (2)	0·33 (3)
In(6)	0·621 (2)	0·364 (2)	0·518 (2)	0·26 (3)
Cu(1)	0	0	0	0·35 (8)
Cu(2)	0·5	0	0	0·34 (8)
Cu(3)	0·061 (4)	0·855 (4)	0·304 (4)	0·29 (6)
Cu(4)	0·696 (4)	0·541 (4)	0·843 (4)	0·26 (6)
Cu(5)	0·772 (4)	0·428 (4)	0·153 (4)	0·33 (6)
Cu(6)	0·866 (4)	0·294 (4)	0·444 (4)	0·28 (6)
Cu(7)	0·582 (4)	0·850 (4)	0·273 (4)	0·31 (6)
Cu(8)	0·838 (4)	0·998 (4)	0·339 (4)	0·33 (6)
Cu(9)	0·664 (4)	0·143 (4)	0·245 (4)	0·28 (6)
Cu(10)	0·654 (4)	0·694 (4)	0·539 (4)	0·36 (6)
Cu(11)	0·713 (4)	0·240 (4)	0·856 (4)	0·25 (6)
Cu(12)	0·251 (4)	0·019 (4)	0·033 (4)	0·27 (6)
Cu(13)	0·437 (4)	0·450 (4)	0·773 (4)	0·24 (6)
Cu(14)	0·866 (4)	0·587 (4)	0·471 (4)	0·25 (6)
Cu(15)	0·915 (4)	0·235 (4)	0·069 (4)	0·34 (6)

Table 2. In–In *and* In(1)–Cu *bond lengths* (Å)

In(1)–In(1)	3·12 (3)	In(1)–Cu(3)	3·04 (4)
–In(4)	3·53 (3)	–Cu(4)	2·73 (4)
–In(5)	3·59 (3)	–Cu(5)	2·75 (3)
In(2)–In(2)	3·27 (4)	–Cu(5)	2·81 (4)
–In(3)	3·16 (2)	–Cu(6)	2·91 (3)
–In(5)	3·49 (3)	–Cu(6)	2·77 (3)
–In(6)	3·38 (3)	–Cu(11)	2·64 (4)
In(3)–In(4)	3·49 (3)	–Cu(14)	2·71 (4)
–In(6)	3·41 (2)	–Cu(14)	2·62 (4)
In(4)–In(5)	3·19 (2)	–Cu(15)	2·78 (4)
		–Cu(15)	2·85 (3)

Discussion. The analysis confirms that the formula of the δ phase is Cu_7In_3 rather than Cu_9In_4. As can be seen in Fig. 1, the In atoms and some of the Cu atoms are arranged in approximate layers parallel to $(\bar{1}30)$. Between these layers, there are layers of Cu atoms. It is interesting to note how the pseudosymmetry arises. The interplanar spacing of $(\bar{1}30)$ is 3·04 Å, which is $\frac{1}{3}$ of the cell parameter of the pseudocubic cell. Indeed, a regular stack of three of the described In layers can be discerned. The planes $(\bar{1}30)$, $(1\bar{3}0)$, (301), $(\bar{3}0\bar{1})$, $(\bar{1}02)$ and $(10\bar{2})$ are approximately perpendicular and they all have a spacing of 3·02–3·04 Å. If these planes are considered as {300} of an orthogonal cell, this cell can

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35645 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

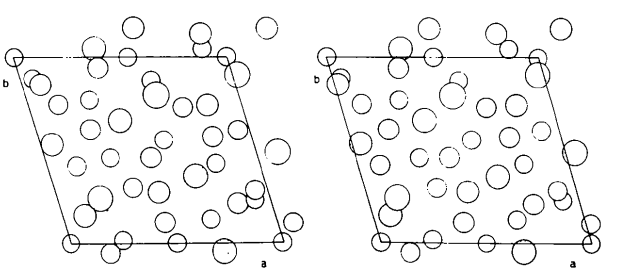

Fig. 1. Stereoplot of Cu_7In_3 on (001). The In atoms are dotted.

be shown to have approximate cubic symmetry. Actually, this transformed cubic unit cell resembles the cubic structure of γ-brass, with cell parameter $a_0 = 8{\cdot}87$ Å, in which most of the atoms are found in positions with x = approximately 0, $\frac{1}{6}$ or $\frac{1}{3}$ (Brandon, Brizard, Chieh, McMillan & Pearson, 1974).

In(1), In(3), In(4) and In(5) are surrounded by 3 In and 11 Cu atoms. In(2) and In(6) also have 11 Cu neighbours, but 4 In and 2 In neighbours respectively. The average In–In distance is 3·38 Å, and the average In–Cu 2·80 Å. These values agree well with accepted values for the atomic radii. The Cu atoms generally have 12 neighbours, 4 or 5 of them being In atoms. The distances between Cu atoms range from 2·50 to 3·0 Å, with an average of 2·73 Å, a value which is significantly larger than the Cu–Cu distance in pure Cu metal (2·55 Å). This is understandable since the Cu atoms have 12 neighbours, as in close-packing; however, some of these neighbours are the bulky In atoms.

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