

bond distances longer than those in the *trans* isomer (Jamet-Delcroix, 1973), as well as the mean value $1.472 (\pm 5) \text{ \AA}$ found in different structures (Kennard *et al.*, 1972). The nitrogen lone pair orbitals point towards Au as suggested by the roughly tetrahedral bond distribution around the N atoms and the Au–N–C bond angles, 108.3° and 109.2° , at N(1) and N(2) respectively.

The enantiomeric anions and the ethylenediammonium cations are packed in three distinct sheets stacked parallel to (100). The components of a given sheet are all identical and equivalent through the *b* and *c* displacements. The sheets containing the aurate ions are related by centres of inversion and are separated, in pairs, by interleaved ethylenediammonium ions. The planar anionic moieties are piled up along [100], their mean plane forming an angle with *a*. In this direction, the Au atoms are located at the vertices of infinite zig-zag chains and subtend an angle of 159.9° ; the metal atoms are alternately separated by distances of 3.846 and 4.254 \AA , indicative of no interaction.

A three-dimensional network of hydrogen bonds is mainly responsible for the cohesion of the crystal lattice, as pictured stereoscopically in Fig. 3. A list of the possible hydrogen-bonded contacts is given in Table 4. All oxygen and hydrogen atoms, except H(9), are involved in hydrogen bonding. The H(9)···O(4) distance of 2.836 \AA and the N(3)···O(4) distance of 3.373 \AA are slightly longer than the sum of the corresponding van der Waals radii. Apart from a slight lengthening of the N···O distances, the hydrogen

bond contraction is still operating despite the sharing of H(10) by two oxygen atoms of one sulphito group and the resulting small H···O–S angles of about 90° . In the *a* direction the sulphito groups are linked through hydrogen bonds with the amino groups of ethylenediamine, whereas bonding with H atoms of the quaternary N atoms determines the packing in the (100) planes.

We thank Dr A. Meyer and Dr S. Losi of Oxy Metal Finishing International, Geneva, Switzerland, for suggesting this problem and supplying the crystals, and Dr S. Losi for assistance in the preliminary determination of the crystal data.

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Acta Cryst. (1975). **B31**, 374

Intermetallic CoIn₂, a Representative of the CuMg₂ Structure Type

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(Received 8 July 1974; accepted 9 September 1974)

CoIn₂ prepared at 500°C crystallizes with the CuMg₂ structure type, space group *Fddd*. The unit cell has edge lengths $a=9.402$, $b=17.846$, and $c=5.282 \text{ \AA}$ and contains 48 atoms. Least-squares refinement of the structural parameters furnished atomic coordinates and bond lengths that were tested against a mathematically rigorous structure model based on hard-sphere contact. The model assumes spherical packing of all atoms of only two diameters and has axial ratios $a/b = \frac{1}{2}$ and $c/b = \frac{1}{3}\sqrt{3}$ and a packing density of 0.68. The agreement with the model is good; the deviations of the observed structure from the model are attributed to preferential Co–In bonds. Bonding in the other known representatives of the CuMg₂ type is also investigated.

Introduction

CoIn₂ was established as a stable phase composition by Schöbel & Stadelmaier (1970). They showed that the phase crystallizes peritectically at 550°C and (wrongly) reported the Bravais lattice as monoclinic.

Meanwhile the lattice was found to be orthorhombic with cell parameters suggesting the CuMg₂ structure type (Ekwall & Westgren, 1940; Schubert & Anderko, 1951). Unlike the related CuAl₂ structure type, which seems ubiquitous, the CuMg₂ type is rarely observed. Beside CuMg₂ itself, only NbSn₂ (Gomes de Mesquita,

Langereis & Leenhouts, 1963) is known to crystallize with this structure type. The interstitial phases Mn_4B (Kiessling, 1950) and Cr_4B (Bertaut & Blum, 1953) may also be classified along with this type. These are defect structures of $CuMg_2$ in which half of the small-atom sites are unoccupied. Interstitial $(CrFe)B$ (Brown & Beerntsen, 1964) is actually isotypic with $CuMg_2$. The present work results from our interest in this structure as a good example of spherical packing, from the possibility of comparing its structural elements with $CoIn_3$ (Stadelmaier, Schöbel, Jones & Shumaker, 1973), and from its relation to the interstitial borides with cubic antiprismatic coordination around the boron, which have been studied in this laboratory for some time (Stadelmaier, 1969).

Sample preparation and composition

Crystals of $CoIn_2$ were grown by reacting solid cobalt (99.74 wt. % purity) with liquid indium (99.99 wt. % purity) for 200 h at 500°C in evacuated capsules of fused silica and quenching to room temperature. This was followed by leaching out the indium matrix with dilute HCl to isolate the $CoIn_2$ particles. The composition of these crystallites was determined as 34.1 ± 0.5 at. % Co and 65.9 ± 0.5 at. % In, using a microprobe analysis, essentially as described by Stadelmaier *et al.* (1973). The composition is also supported by the agreement between the measured density and the X-ray density, assuming 16 cobalt and 32 indium atoms per unit cell, and, of course, by the structure analysis.

Experimental

Rotation patterns about the cell axes fixed the approximate cell constants. The final cell constants were obtained from powder patterns taken in a Straumanis type camera (diameter 114.59 mm), using $Co K\alpha_1$, $\lambda = 1.78892 \text{ \AA}$ and $Co K\alpha_2$, $\lambda = 1.79278 \text{ \AA}$ in the back reflection region and extrapolating to $\theta = 90^\circ$. Better precision could have been reported for the cell constants by using reflections from the whole angular range, but

it is felt that the extrapolation accounts better for the camera errors. The single-crystal integrated intensities of 399 reflections were collected on a manually operated Picker four-circle diffractometer using the 2θ -scan method and sampling one octant in reciprocal space limited by $0 < 2\theta < 70^\circ$. $Mo K\alpha$ radiation passed over a perpendicular quartz ($10\bar{1}1$) monochromator was employed. The standard Lp correction was used since the additional polarization from the monochromator is small. Because the crystal had the shape of an equiaxed polyhedron, the intensities were further adjusted through the spherical absorption correction given in *International Tables for X-ray Crystallography* (1967). A μR of 4.4 was used, corresponding to transmission factors A between 0.009 and 0.033 for the observed reflections. The data for the orthorhombic cell of $CoIn_2$ are $a = 9.402 \pm 0.005$, $b = 17.846 \pm 0.011$, $c = 5.282 \pm 0.003 \text{ \AA}$, $a/b = 0.5268$, $c/b = 0.2960$, $V = 886.3 \text{ \AA}^3$, $D_m = 8.68 \pm 0.17$, $D_x = 8.65 \text{ g cm}^{-3}$, $M = 16$.

Verification of the $CuMg_2$ structure and refinement of the parameters

The observed single-crystal reflections obeyed the conditions hkl : $h+k$, $k+l=2n$, $h+k+l=2n+1$ or $4n$; $h0l$: $l+h=4n$; $hk0$: $h+k=4n$. There were two exceptions: forbidden reflections 886 and 2,12,4, which were weak, had irregular peak profiles and are presumed to be double reflections. The systematic extinctions are satisfied by the centrosymmetric space group $Fddd$ (No. 70). For the structure calculations the CRYM crystallographic computing system (Duchamp, 1964) was used. The $CuMg_2$ arrangement was readily verified and refined by a full-matrix, least-squares method in which the function minimized was $\sum w^2(|F_o|^2 - |F_c/k|^2)^2$. The weights w were provided through a Hughes $1/F_o^2$ weighting scheme. In the final refinement cycles 14 adjustable parameters (three positional, nine anisotropic temperature parameters U_{ii} , one extinction parameter g , and one scale factor k) were fixed by 374 non-zero reflections, or 27 data per parameter. Orthogonal vibrational amplitudes U_{ii} were included for

Table 1. Final parameters ($\times 10^4$) of $CoIn_2$ with *e.s.d.*'s

$U_{ii} \times 10^4$ in \AA^2 . Origin at I.

	Number	Position	X/a	Y/b	Z/c	U_{11}	U_{22}	U_{33}
In(1)	16	(e)	9649 (2)	1250 (0)	1250 (0)	181 (6)	116 (6)	187 (7)
In(2)	16	(f)	1250 (0)	7131 (1)	1250 (0)	176 (6)	155 (7)	165 (7)
Co	16	(f)	1250 (0)	9971 (2)	1250 (0)	173 (11)	81 (10)	132 (11)

Secondary extinction factor $g \times 10^6$: 1.33 (9)

Table 2. Coordinates of $CoIn_2$ transformed to $CuMg_2$ setting and compared with $CuMg_2$ coordinates

$CoIn_2$ axes permuted to *cab* and origin shifted to 222.

Position		X/a	Y/b	Z/c	X/a	Y/b	Z/c
(f)	In(1)	0	0.1601	0	Mg(1)	0	0.161
(g)	In(2)	0	0	0.4119	Mg(2)	0	0.411
(g)	Co	0	0	0.1279	Cu	0	0.128

each of the three site sets. (Symmetry restrictions cause two of the $U_{ij}(i \neq j)$ in each site set to be zero and the remaining ones, U_{23} for position (e) and U_{31} for (f), are negligibly small.) The fit was further improved by using secondary extinction corrected F_c^2 values given by $F_c^2/(1 + \beta g F_c^2)$, following the description of Larson (1967) where g is the extinction factor and β a function of Bragg 2θ . The absorption dependence of β is neglected in this treatment.

The structural parameters found for CoIn₂ are listed together with their e.s.d.'s (in parentheses) in Table 1. Because our origin was located at a center of symmetry and our axes follow the convention $c < a < b$, we have also transformed the atomic coordinates to the setting of Ekwall & Westgren (1940) in Table 2. The coordinates of CuMg₂ as given by Schubert are included for comparison. Twenty-five unobserved reflections were excluded from the refinement but included in the unweighted reliability index $R = \sum |k|F_o| - |F_c| / \sum k|F_o|$. The final R was 0.068 for 399 reflections.* A three-dimensional difference Fourier map was reasonably flat, the maximum difference between ρ_o and ρ_c being $3 \text{ e } \text{Å}^{-3}$.

Geometry of the CuMg₂ type

Various views of the CuMg₂ structure, which will not be repeated in detail, can be found in one of the following references: Ekwall & Westgren (1940), Schubert & Anderko (1951), Schubert (1964), Pearson (1972); for Mn₄B, Kiessling (1950). Schubert & Anderko revealed the relation to CuAl₂ and NiMg₂ through the observation that the small atoms are inside square antiprisms formed by large atoms. The antiprisms are stacked along [101] in such a way that each square is shared by two contiguous polyhedra. Consequently, each center atom has eight large neighbors and two small neighbors, the latter being located on the prism axis. For Mn₄B this coordination around the small atom remained unrecognized for some time, but Goldschmidt (1967) was definitely aware of it. Kiessling (1950) emphasized the many near-regular tetrahedra, a structural element generally found in close-packed arrangements. The nearly regular hexagonal nets on (010) planes (our notation) are described by Bertaut & Blum (1953) for Cr₄B, Schubert (1964) for CuMg₂, and Brown & Beerntsen (1964) for (CrFe)B. The hexagons were missed by Ekwall & Westgren (1940) who believed that the a/c ratio near $\sqrt{3}$ found by Grime & Morris-Jones (1929) was accidental.

In metallic compounds it is usually not difficult to relate an apparently complex structure to the close packing of rigid spheres. We have investigated this for the CuMg₂ type and found that a mathematically rig-

orous but elementary analysis, based on a few plausible premises, leads to the correct axial ratios and fractional atomic coordinates. The basic assumptions and their consequences are detailed in the following: (a) There are only two atomic diameters, one for indium, and a smaller one for cobalt. The hexagonal rings of indium on (010) are regular and all of their spherical atoms touch. From this follows $a/c = \sqrt{3}$, and the In(1) parameter $X/a = \frac{2}{3} - \frac{1}{6} = 0.9583$ (our notation) or $Y/b = \frac{1}{6} = 0.1667$ (Westgren's notation). (b) Along [010] the spacing between hexagonal layers is uniform. Then the In(2) parameter must be $Y/6 = \frac{7}{6} - \frac{1}{6} = 0.7083$ (our notation) or $Z/c = \frac{1}{4} + \frac{1}{6} = 0.4167$ (Westgren's notation). (c) The tetrahedra consisting of In(1) and In(2) are regular and close-packed. From this follows $a/b = \frac{1}{2}$ and also $c/b = \frac{1}{6}\sqrt{3} = 0.2887$. Other properties of this rigid-sphere model are: The cubo-octahedra are not regular, but any intermeshing pair of square faces is twisted out of the ideal 45° configuration by 8° . Hence the radius ratio between a small atom at the center of the antiprism and the large atoms at the vertices is not the ideal $(2 + \frac{1}{2}\sqrt{2})^{1/2} - 1 = 0.6453$ but takes on the larger value $\frac{1}{2}\sqrt{13} - 1 = 0.8028$. This ratio fixes the cobalt diameter in the model. The fractional coordinate Y/b for cobalt is exactly zero (or $\frac{1}{3}$ in Westgren's notation). Finally, the theoretical density, $\sum (\text{sphere volumes}) / (\text{unit-cell volume})$ is $4\pi[2 + (\frac{1}{2}\sqrt{13} - 1)^3] / 27\sqrt{3} = 0.676$. It equals almost exactly the packing density of a body-centered metal (e.g. α -iron), namely $\frac{1}{2}\pi\sqrt{3} = 0.680$. This information is compiled in Table 3, and the observed parameters of the known representatives of this structure type are included for comparison, after conversion to our setting. Spherical packing is undoubtedly a valid description of the structure.

Table 3. Rigid-sphere model

Parameter	Model	CuMg ₂	CoIn ₂	NbSn ₂	B(CrFe)BMn ₄
a/b	5000	4970	5268	5155	5024 5019
c/b	2887	2895	2960	2953	2896 2897
$X/a, \text{In}(1)$	9583	9640	9649	9563	9571 9580
$Y/b, \text{In}(2)$	7083	7140	7131	7076	7070 7080
$Y/b, \text{Co}$	9999	9970	9971	9982	9999 9999
CN12 radius ratio	8028	7985	7929	8971	7729 7729

The observed atomic distances in CoIn₂ are given in Table 4. Their standard deviations include the errors in the cell parameters. Each bond length is characterized by a vector specifying its direction and magnitude in the model. (Most vectors would not have rational components in the real structure.) The model distances, also listed in Table 4, are obtained by using these vectors with the model axial ratios and an indium radius of 1.53 Å. The radius is somewhat arbitrarily chosen to cause the atomic distortions from the spherical shape to be evenly distributed between expansion and contraction. 1.53 also represents the indium radius for

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 30675 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

coordination number 8 when derived from Pauling's (1960) single-bond radius. Based on the strong bonds, the observed coordination number for indium is 7 to 9. It is seen from Table 4 that the expectation of a uniform bond length between cobalt and its eight antiprismatic neighbors is not quite satisfied. The model distances of 3.421 Å are the sides of the squares on the antiprism whereas the shorter 3.060 Å distances link a pair of squares located on opposite sides of the surrounded cobalt atom. In a regular 45° cubic antiprism these two sets of lengths (3.421 and 3.060) would have to be identical, but in the present model they must differ, spherical contact being allowed only for the 3.060 length but not for 3.421. The four vectors with magnitudes 3.060 also represent edges of the regular tetrahedra in the model so that the deviation of the observed bond lengths from 3.060 measures the distortion of the tetrahedra in the real structure.

Bonding in the CuMg₂ family

Table 3 suggests that the distortion against spherical packing is virtually absent in Mn₄B. The observed distortion in CoIn₂ is best interpreted along the lines suggested for CoIn₃ (Stadelmaier *et al.*, 1973) where it was attributed to a strong Co-In bond with a distance of 2.60 Å which, incidentally, is a single bond when the bond number is figured according to Pauling (1960). Looking over the table of distances in the CoIn₃ paper one notes the distances Co-In 2.732 and In-In 2.980, 3.136, 3.316, 3.547, having close counterparts in CoIn₂, Table 4. The stronger of the bonds in CoIn₂ with distances 2.73, 3.00, and 3.14 Å have bond numbers close to the rational fractions $\frac{1}{2}$, $\frac{1}{2}$, and $\frac{1}{3}$. The conclusion must be that in both CoIn₃ and CoIn₂ the distortions are controlled by bonding forces which satisfy Pauling's suggestion that the bond numbers in metallic

Table 4. Atomic distances in CoIn₂ (Å)

Reference atom	Neighbor	Number of neighbors	Distance	Vector in model	Distance in model	Remarks
Co	Co	2	2.698 (6)	[101]/4	2.650	Cubic antiprism
	In(1)	2	2.684 (14)	[236]/24	2.758	
	In(1)	2	2.734 (16)	[430]/24	2.758	
	In(2)	2	2.735 (5)	[0,1,12]/24	2.758	
	In(2)	2	2.763 (9)	[616]/24	2.758	
In(1)	Co	2	2.684 (14)	[236]/24	2.758	Hexagonal ring
	Co	2	2.734 (16)	[430]/24	2.758	
	In(1)	1	3.010 (8)	[100]/3	3.060	
	In(1)	2	3.136 (6)	[103]/6	3.060	
	In(2)	2	3.287 (17)	[123]/12	3.421	
	In(2)	4	3.422 (10)	[216]/12	3.421	
	In(2)	2	3.562 (13)	[410]/12	3.421	
In(2)	Co	2	2.735 (5)	[0,1,12]/24	2.758	
	Co	2	2.763 (9)	[616]/24	2.758	
	In(1)	2	3.287 (17)	[123]/12	3.421	
	In(1)	4	3.422 (10)	[216]/12	3.421	
	In(1)	2	3.562 (13)	[410]/12	3.421	
	In(2)	2	3.001 (9)	[313]/12	3.060	
	In(2)	1	3.144 (7)	[010]/6	3.060	

Table 5. Bonding electrons associated with atoms equivalent to In(1)=A(1) and In(2)=A(2)

Small atom is B. D_n is observed distance at bond number n . Total = \sum (number of neighbors $\times n$).

Atom	Neighbors	CuMg ₂		CoIn ₂		NbSn ₂		B(CrFe)	
		D_n	n	D_n	n	D_n	n	D_n	n
A(1)	2B	2.695	0.55	2.684	0.68	2.945	0.50	2.195	0.42
	2B	2.755	0.44	2.734	0.56	2.948	0.50	2.210	0.40
	1A(1)			3.010	0.53	3.160	0.30	2.389	0.88
	2A(1)			3.136	0.32	3.271	0.19	2.456	0.68
	2A(2)							2.708	0.26
	4A(2)							2.718	0.25
	2A(2)							2.734	0.23
Total, A(1)			1.98		3.65		2.68		5.86
A(2)	2B	2.695	0.55	2.735	0.56	2.862	0.68	2.164	0.47
	2B	2.735	0.47	2.763	0.50	2.941	0.51	2.222	0.38
	2A(2)			3.001	0.54	3.247	0.21	2.427	0.76
	1A(2)			3.144	0.31	3.327	0.16	2.460	0.67
	2A(1)							2.708	0.26
	4A(1)							2.719	0.25
	2A(1)							2.734	0.23
Total, A(2)			2.04		3.51		2.96		5.87
Pauling valence of A			2.00		3.56		2.56		6.00

compounds prefer ratios of small integers. The bond numbers for four compounds, calculated from $-\log n = (D_n - D_1)/0.6$, are listed in Table 5, the list terminating when the bonding electrons on the reference atom are exhausted, *i.e.*, when the bond numbers times the number of neighbors add up to the Pauling (1960) valence. One will note that three quarters of the bond numbers are reasonably close to the fractions $\frac{3}{4}, \frac{2}{3}, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}$. The spatial distribution of bonding electrons around the large atom suggested by Table 5 has the following meaning. There can be no strong attraction between magnesium atoms in CuMg_2 ; the structure is held together by Cu-Cu and Cu-Mg bonds. In CoIn_2 and NbSn_2 , the strong bonds to the large reference atom lie within the first coordination shell of seven near neighbors. The atoms remaining outside this shell are the same ones that make no hard-sphere contact in the model structure. In the interstitial boride, the metal atoms appear to be bonded to all of the 15 closest neighbors. The strongest bonds (highest bond numbers) are found between large-atom pairs, *i.e.*, metal-atom pairs, not between the large and small atom, *i.e.*, metal atom and boron. This tends to confirm the long held view of the metal-rich interstitial compound that it consists of a substantially metallic framework stabilized by the insertion of small metalloid atoms.

Incidentally, the indium atoms are located at the center of CN 15 μ -phase polyhedra, and another way to develop the structure is by stacking such polyhedra down the long axis [010] in the manner of Samson's (1968) description of complex structures by the packing of coordination polyhedra.

A brief remark concerning the thermal parameters in CoIn_2 follows. An ellipsoid cannot be expected to describe the thermal motion under the influence of the seven bonds to an indium atom or the eight bonds to cobalt. The restrictions on the thermal parameters mentioned above and imposed by having the special position atoms (*e*) and (*f*) located on rotation diads [see Levy (1956)], would only seem to make matters worse. That the U_{ii} are nevertheless susceptible to physical interpretation is seen by considering U_{22} of

cobalt in the [010] direction (Table 1). Its low value correlates with the observation that fully half of the eight cobalt neighbors, namely all In(1), have bond vectors whose resultants parallel [010] and $[0\bar{1}0]$. Furthermore, the bonds between Co and In(1) are the strongest in the structure.

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