

atoms. However, besides the higher C content of UMoC_2 , the C positions of $\text{Ho}_2\text{Cr}_2\text{C}_3$ do not all correspond to the occupied positions in UMoC_2 , although the arrangements of the metal atoms correspond in the two structures. The compounds $\text{U}_2\text{Mo}_2\text{C}_3$ and $\text{U}_2\text{W}_2\text{C}_3$ are isotypic with $\text{Ho}_2\text{Cr}_2\text{C}_3$. This also appears to be the case for the compound $\text{PuWC}_{1.75}$ (Ugajin, Abe, J. Nucl. Mater. (1973) 47, 117).

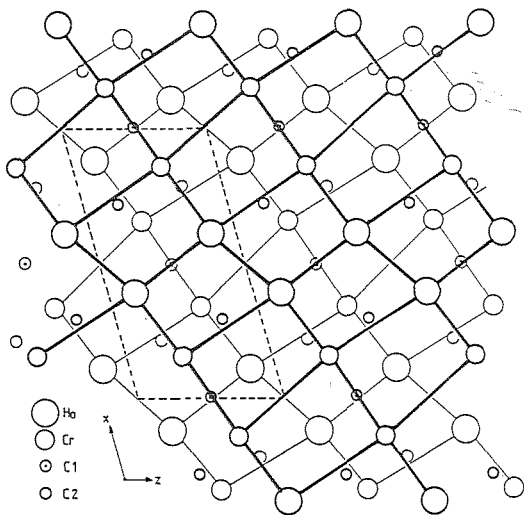


Fig. 1. Crystal structure of $\text{Ho}_2\text{Cr}_2\text{C}_3$. Atoms connected by thick and thin lines are at $y = 0$ and $y = 1/2$ respectively.

08.3-6 $\text{Pr}_2\text{Mn}_{17}\text{C}_{3-x}$, A COMPLEX CARBIDE WITH FILLED $\text{Th}_2\text{Zn}_{17}$ STRUCTURE. By G. Block and W. Jeitschko, Anorganisch-Chemisches Institut, Universität Münster, D-4400 Münster, West Germany.

The title compound was prepared by reaction of the elemental components in a high frequency furnace with subsequent annealing at 800 °C. It crystallizes with a rhombohedral cell, space group $R\bar{3}m$ and the hexagonal lattice constants: $a = 8.8714(7) \text{ \AA}$, $c = 12.783(2) \text{ \AA}$, $V = 871.2 \text{ \AA}^3$, $Z = 3$. The structure was determined from single crystal X ray data and refined to a residual of $R = 0.023$ for 25 variable parameters and 414 independent structure factors. The structure can be derived from that of $\text{Th}_2\text{Zn}_{17}$ (Makarov and Vinogradov, Sov. Phys. Crystallogr. (1956) 1, 499) with the Pr and Mn positions corresponding to those of Th and Zn. The carbon atoms fill octahedral voids formed by a square of Mn atoms (Mn-C distances of 1.94 Å (2x) and 1.95 Å (2x)) and two Pr atoms at 2.57 Å. The ideal composition with all octahedral voids filled is represented by the formula $\text{Pr}_2\text{Mn}_{17}\text{C}_3$. The refinement of the occupancy parameter of the carbon positions, however, showed that these positions are only occupied to 57±3 % in the crystal picked for the structure determination. The Pr atoms are situated in a coordination polyhedron formed by three carbon atoms at 2.57 Å, 19 Mn atoms (at distances varying between 3.19 and 3.43 Å) and one Pr atom at 3.95 Å. The four crystallographically different Mn atoms have coordination numbers 12, 13 and 14 with zero or one C neighbor, one, two or three Pr neighbors and between 9 and 13 Mn neighbors (Fig. 1).

The new compound $\text{La}_2\text{Mn}_{17}\text{C}_{3-x}$ is isotypic with $\text{Pr}_2\text{Mn}_{17}\text{C}_{3-x}$. A compound reported by Stadelmaier and Park (Z. Metallk. (1981) 72, 417) with the composition $\text{Gd}_4\text{Fe}_{31}\text{C}_3$ most likely is isotypic with $\text{Pr}_2\text{Mn}_{17}\text{C}_{3-x}$. The structure will be discussed together with other recent examples of ternary carbides which can be derived from binary structure types by filling of interstitial voids.

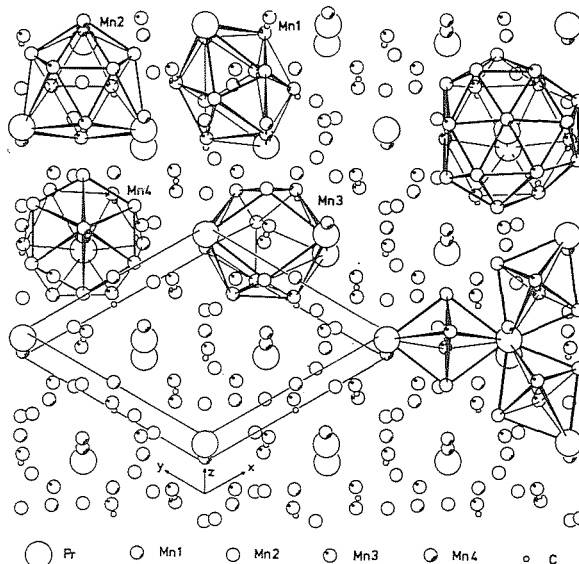


Fig. 1. Coordination polyhedra in $\text{Pr}_2\text{Mn}_{17}\text{C}_{3-x}$. Only one half of the structure between $z = 0$ and $z = 1/2$ is shown.

08.3-7 TEMPERATURE DEPENDENCE OF THE LATTICE CONSTANTS AND THE CRYSTAL STRUCTURE OF $\text{Mn}_{11}\text{Ge}_8$ AT 295 K AND 116 K. By T. Ohba, N. Watanabe and Y. Komura, Faculty of Science, Hiroshima University, Naka-ku, Hiroshima, Japan.

Four intermetallic compounds were reported in Mn-Ge system according to Elliot. Among them Mn_3Ge_2 was found to be antiferromagnet at low temperature and it transforms to weak ferromagnet at 160 K, then changes to a paramagnet at 300 K [Zavadskii and Fakidov; Soviet Physics JETP 24, 887 (1967)].

Israiloff et al. [Monatsh. Chem. 105, 1387 (1974)] studied the crystal structure and concluded that Mn_3Ge_2 is isotypic with $\text{Cr}_{11}\text{Ge}_8$ by a comparison of the powder pattern. In this paper, the crystal structure of $\text{Mn}_{11}\text{Ge}_8$ is refined by a single crystal X-ray diffraction method at 295 K and 116 K. Crystal Data: Orthorhombic, Pnam, $a=13.214(2)$, $b=15.880(3)$ and $c=5.0905(5) \text{ \AA}$, $Z=4$ at 295 K.

The temperature dependence of the lattice constants is measured using a single crystal. Fig. 1 shows a curve for lattice constant a vs temperature for an example. A kink appears at the transition temperature (160 K). Kinks are also observed on curves for b - and c -axis at the same temperature.

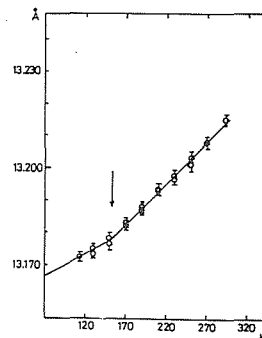


Fig. 1

The refinement of the structure was made at 295 K and 116 K using a program RADIEL [Coppens et al.; Acta Cryst. A35, 63 (1979)]. The final weighted R(F) values are 0.0292 and 0.0260 at 295 K and 116 K, respectively. Although the crystal symmetry does not change, the positional parameters above and below the transition temperature show non-uniform changes of the interatomic distances. The histograms of the change of the interatomic distances ($\Delta d = d_{295} - d_{116}$) for Ge-Ge, Mn-Ge and Mn-Mn are shown in Fig. 2. Changes of the Mn-Mn distances are greater than those of Mn-Ge and Ge-Ge, and some of Mn-Mn distances are even expanded at 116 K. Such features of the interatomic distances suggest that the contribution of Mn-Mn distances to the magnetic property is fairly large in $Mn_{11}Ge_8$. The deformation densities along Mn-Mn bonds, which are expanded at 116 K, vary considerably from 295 K to 116 K.

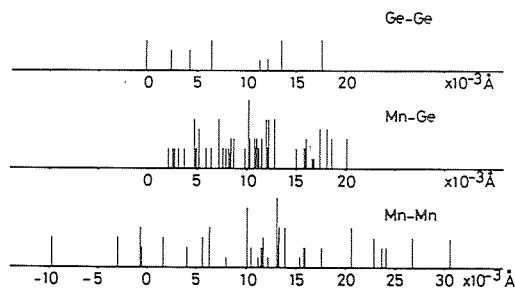


Fig. 2

08.3-8 CRYSTAL STRUCTURE OF $Pr_6Ni_7Si_4$, AN INTERGROWTH OF THREE SIMPLER STRUCTURAL SLABS. By E. Hovestreydt and E. Parthé, Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24, quai Ernest Ansermet, CH-1211 Genève 4 (Switzerland).

$Pr_6Ni_7Si_4$ crystallizes with an orthorhombic unit cell (oP68, Pbcm, $a = 5.888(1)$, $b = 7.4265(9)$, $c = 29.558(8)$ Å). Its structure corresponds to a new structure type which can be described as an intergrowth of three types of slabs. One has an arrangement of Ni centered trigonal Pr prisms as in the Fe_3C type, which is already found with Pr_2Ni . The second slab can be described as a segment of a $ThSi_2$ type structure also with trigonal Pr prisms which are centered by Ni atoms. The $ThSi_2$ type has not yet been found with binary rare earth transition metal compounds, however, a ternary variant occurs with $PrNiSi$. The third slab which is only 3 Å thick and contains Pr, Ni and Si atoms lies between the $ThSi_2$ and the Fe_3C type slabs. The atom arrangement in the thin slab has similarities with the $TiNiSi$ type, a $PbCl_2$ derivative type, which is found for example with $PrNiGa$. However, the coordination polyhedra of the Ni and Si atoms in this thin slabs include Pr atoms from the neighbouring slabs. All Ni and Si atoms are thus found to be in the centers of strongly deformed trigonal Pr prisms.

An isotopic phase seems to exist in the system Ce-Ni-Si where M.G. Mis'kiv (thesis, Ivano Franko Univ., Lvov, USSR, 1973) found a compound with similar lattice constants and space group, however, the composition given there was $Ce_{10}Ni_{12}Si_3$.

A detailed account of this structure determination will be published in Acta Crystallographica.

08.3-9 THE CRYSTAL STRUCTURE OF $Co_2P(h)$ AND ITS

STRUCTURAL RELATIONSHIP TO THE $Co_2P(r)$.

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In the system Co-P, the following compounds are known: Co_2P (Ni_2Si type), CoP (MnP type) and CoP_3 ($CoAs_3$ type). The metallographic investigation showed that the compound Co_2P undergoes a phase transformation. The X-ray powder investigation confirms the polymorphism of Co_2P . The since known compound Co_2P isostructural to Ni_2Si (Nowotny, Z. anorg. Chem. (1947) 254, 349; Rundquist, Acta Chem. Scand. (1960) 14, 1961) is the low-temperature form $Co_2P(r)$. The new high-temperature phase $Co_2P(h)$ stable at above 1400K is isostructural to Fe_2P . The crystal powder data of the high-temperature phase are:

$Co_2P(h)$, $P\bar{6}2m$, Fe_2P type, $a = 5.722(1)$, $c = 3.476(1)$ Å

Among all the homologous phases isostructural to Fe_2P , $Co_2P(h)$ shows the highest axial ratio $c/a = 0.607$.

The other crystal chemical data of compounds isostructural to Fe_2P , and Ni_2Si will be compared with the data of $Co_2P(h)$ and $Co_2P(r)$. The structural relationship between the Fe_2P and Ni_2Si type structure will be discussed.

08.3-10 $Zr_2Ru_3Si_4$, A NEW STRUCTURE TYPE CONTAINING COLUMNS OF SHARED Si-CENTERED ANTIPRISMS AND OF SHARED Ru-CENTERED OCTAHEDRA. By B. Chabot†, E. Parthé† and H.F. Braun††. †Laboratoire de Cristallographie aux Rayons X, Université de Genève, ††Département de Physique de la Matière Condensée, Université de Genève, 24, quai Ernest Ansermet, CH-1211 Genève 4, Switzerland.

$Zr_2Ru_3Si_4$ crystallizes with a monoclinic unit cell (mC72, $C2/c$) with $a = 18.992(3)$, $b = 5.3476(8)$, $c = 13.289(3)$ Å and $\beta = 127.73(1)^\circ$. Its structure corresponds to a new structure type which is characterized by

- columns of Si-centered face-shared square antiprisms formed by Zr and Ru atoms
- columns of Ru-centered face-shared Si-octahedra.

Columns of centered antiprisms and columns of centered octahedra are structural features which are found in other ternary compounds $R_xT_yM_z$ where R is an early transition element (Sc, Ti, Zr, Hf) or a small rare-earth (Lu); T is a transition element of the Cr, Mn, Fe or Co group and M is Si or Ge atom. The compositions of these structures can be related to :

- the composition of the M-centered antiprism columns ($R_4T_4M_2$ or $R_6T_2M_2$ or R_8M_2)
- the type of linkage of the T-centered M-octahedron columns (isolated column : M_6T_2 ; edge-linked to two other columns : $M_2M_4/2T_2$, or edge-linked to three other columns : $M_{6/2}T_2$)
- the presence or not of additional Si atoms inbetween the antiprism columns.

In the table, calculated stoichiometries and formulae of known structure types are shown as a function of anti-