

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.

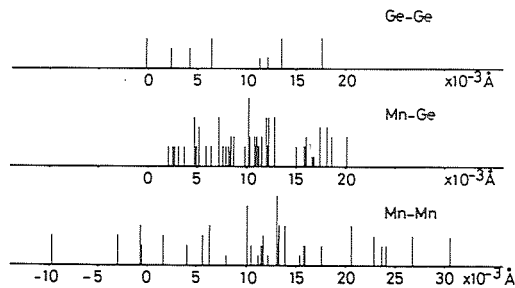


Fig. 2

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 isotypic 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-