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 (d=s-1, d=1) 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 Mn1,Ge. The deformation densities along Mn-Mn bonds, which are expanded at 116 K, vary considerably from 295 K to 116 K.

![Fig. 2](image-url)

### 08.3-9 THE CRYSTAL STRUCTURE OF Co2P(h) AND ITS STRUCUTRAL RELATIONSHIP TO THE Ce2P(r)

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In the system Co-P, the following compounds are known: Co2P (Ni2Si type), CoP (MnP type) and Co3P (CoAs type). The metallographic investigation showed that the compound Co2P undergoes a phase transformation. The X-ray powder investigation confirms the polymorphism of Co2P. The known compound Co2P is isomorphous to Ni2Si (Nowotny, Z. anorg. Chem. (1947) 234, 349; Rundquist, Acta Chem. Scand. (1960) 14, 1961) is the low-temperature form Co2P(r). The new high-temperature phase Co2P(h) is stable at about 1400 K and is isomorphous to Fe2P. The crystal powder data of the high-temperature phase are:

- Co2P(h), P63m, Fe2P type, a = 5.722(1), c = 3.476(1) Å
- Among all the homologous phases isomorphic to Fe2P, Co2P(h) shows the highest axial ratio c/a = 0.607.

The other crystal chemical data of compounds isomorphous to Fe2P, and Ni2Si will be compared with the data of Co2P(h) and Co2P(r). The structural relationship between the Fe2P and Ni2Si type structure will be discussed.

### 08.3-10 Zr2Ru3Si4, A NEW STRUCTURE TYPE CONTAINING COLUMNS OF SHARED SI-CENTERED ANTIPRISMS AND OF SHARED Ru-CENTERED OCTAHEDRA

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Zr2Ru3Si4 crystallizes with a monoclinic unit cell (mC72, C2/c) with a = 18.092(3), b = 5.347(6), c = 13.289(3) Å and β = 111.73(1)°. 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 R2TM, where R is an early transition element (Sc, Ti, Zr, Hf) or a 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 antiprisms columns (R2T2M2 or R2T2M'2 or R2T2)
- the type of linkage of the T-centered M-octahedron columns (isolated column : M2T2 ; edge-linked to two other columns : M2T2M2, or edge-linked to three other columns : M2T2M4)
- the presence or not of additional Si atoms inbetween the antiprisms columns.

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