The crystal structures of the new compound \( \text{YCo}_3\text{P}_3 \) were prepared by the tin flux technique. Their structure was determined from X-ray data and refined to a residual of \( R = 0.051 \) for 908 unique structure factors and 30 variable parameters.

Single crystals of the new compound \( \text{LaCo}_3\text{P}_5 \) were grown by reaction of the elemental components in a tin flux. They have orthorhombic symmetry: \( a = 10.501(3) \text{ Å}, b = 3.596(1) \text{ Å}, c = 9.343(2) \text{ Å}, V = 352.8 \text{ Å}^3 \), space group \( \text{Pmnn} \), \( Z = 2 \). The structure was determined by direct methods and refined to a residual of \( R = 0.040 \) for 49 variable parameters and 927 unique \( F \) values. It belongs to a large family of structures of which the ternary equiatomic structures of the \( \text{Fe}_3\text{P} \) and \( \text{TiNiSi} \) type are considered as the most simple representatives. These structures are usually characterized by the arrangement of the coordination polyhedra of the metalloid atoms. These polyhedra consist of trinodal prisms of metal atoms which are augmented by three additional atoms outside the rectangular faces of the prisms. The polyhedra have a coordination number of 18 whereas the \( \text{La}_3\text{Co}_2\text{P}_3 \) and \( \text{La}_3\text{Co}_2\text{P}_3 \) have coordination number 21.

The coordinates of \( \text{La}_{16}\text{Co}_{32}\text{P}_{48} \) are given in Table 1. The structure is of a new type (Fig. 1). While the compounds with a metal:metalloid ratio of \( 2:1 \) (e.g. \( \text{LaCo}_3\text{P}_5 \)) the trinodal prisms share only edges, in \( \text{LaCo}_3\text{P}_5 \) with a slightly lower metal content some of the prisms share also faces (Fig. 1). When the compounds with a metal:metalloid ratio of \( 2:1 \) have no metalloid-metalloid bonds, the lower metal content results in a short \( P-P \) distance of 2.40 \( \text{Å} \), which is formed across the common face of the face-sharing prisms. The La atoms have a large coordination number: 8 P (3.09 and 3.15 \( \text{Å} \)) and 9 Co (from 3.08 to 3.34 \( \text{Å} \)) and 2 La at 3.60 \( \text{Å} \). There are five different sites which correspond to the sites of the large tetrahedra of the \( \text{LaCo}_3\text{P}_5 \) structure. In three of these the Co atoms have a coordination of 8 metal and 4 P atoms. These sites correspond to the sites of the small transition metal atoms in the \( \text{LaCo}_3\text{P}_5 \) and \( \text{TiNiSi} \) type structures. There it is sometimes called the tetrahedral site, because the four P neighbors form distorted tetrahedra. One Co atom has a coordination of 10 metal and 5 P atoms. The latter form a square pyramid. It corresponds to site a of the large tetrahedra in the ternary \( \text{P} \) and \( \text{TiNiSi} \) type structures. The thermal parameters of the Co atoms correlate with the coordination numbers: large thermal amplitudes are observed for sites with large coordination numbers. This is also the case in related structures as in \( \text{ErCo}_3\text{P}_3 \) and \( \text{Er}_2\text{Ni}_12\text{P}_7 \) (Jeitschko and Jaberg, Z. Anorg. Allg. Chem. (1980) 467, 95) and \( \text{Nd}_2\text{Ni}_12\text{P}_7 \) (Guéritin, Potel, Sergent, J. Less-Common Met. (1981) 78, 177).

Fig. 1. Comparison of the crystal structures of \( \text{LaCo}_3\text{P}_5 \) and \( \text{LaCo}_3\text{P}_5 \). The trigonal prisms of metal atoms (large circles: \( \text{La} \), small circles: \( \text{Co} \) around the \( P \) atoms (filled circles) are emphasized. Atoms connected by thin and thick lines are separated from each other by half a translation period of the projection direction.

Fig. 2. Similarities of the structures of \( \text{YCo}_3\text{P}_3 \), \( \text{LaCo}_3\text{P}_5 \), and \( \text{YNi}_3\text{Si}_3 \) (\( \text{YNi}_3\text{Si}_3 \) type). The trigonal prisms of metal atoms (large and small circles for the rare earth and transition metals respectively) around the metalloid atoms (black dots) are emphasized. Atoms connected by thin and thick lines are separated from each other by half a translation period of the projection direction.

Fig. 1. Crystal structure and near-neighbor coordinations of \( \text{YCo}_3\text{P}_3 \). Atoms connected by thin and thick lines are at \( y = 1/4 \) and \( 3/4 \) respectively. The coordination polyhedra all have mirror planes perpendicular to the projection direction.

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08.3-13 TERNARY LANTHANOID IRON AND COBALT PHOSPHIDES WITH THE NEW \( \text{YCo}_3\text{P}_3 \) TYPE STRUCTURE. By W. Jeitschko and U. Meisen, Anorganisch-Chemisches Institut, Universität Münster, D-4400 Münster, West Germany.

Crystals of the new compound \( \text{YCo}_3\text{P}_3 \) were grown by reaction of the elemental components in a tin flux. They have orthorhombic symmetry: \( a = 10.501(3) \text{ Å}, b = 3.596(1) \text{ Å}, c = 9.343(2) \text{ Å}, V = 352.8 \text{ Å}^3 \), space group \( \text{Pmnn} \), \( Z = 2 \). The structure was determined by direct methods and refined to a residual of \( R = 0.040 \) for 49 variable parameters and 927 unique \( F \) values. It belongs to a large family of structures of which the ternary equiatomic structures of the \( \text{Fe}_3\text{P} \) and \( \text{TiNiSi} \) type are considered as the most simple representatives. These structures are usually characterized by the arrangement of the coordination polyhedra of the metalloid atoms. These polyhedra consist of trinodal prisms of metal atoms which are augmented by three additional atoms outside the rectangular faces of the prisms. The polyhedra have a coordination number of 18 whereas the \( \text{La}_3\text{Co}_2\text{P}_3 \) and \( \text{La}_3\text{Co}_2\text{P}_3 \) have coordination number 21.

The coordinates of \( \text{La}_{16}\text{Co}_{32}\text{P}_{48} \) are given in Table 1. The structure is of a new type (Fig. 1). While the compounds with a metal:metalloid ratio of \( 2:1 \) (e.g. \( \text{LaCo}_3\text{P}_5 \)) the trinodal prisms share only edges, in \( \text{LaCo}_3\text{P}_5 \) with a slightly lower metal content some of the prisms share also faces (Fig. 1). When the compounds with a metal:metalloid ratio of \( 2:1 \) have no metalloid-metalloid bonds, the lower metal content results in a short \( P-P \) distance of 2.40 \( \text{Å} \), which is formed across the common face of the face-sharing prisms. The La atoms have a large coordination number: 8 P (3.09 and 3.15 \( \text{Å} \)) and 9 Co (from 3.08 to 3.34 \( \text{Å} \)) and 2 La at 3.60 \( \text{Å} \). There are five different sites which correspond to the sites of the large tetrahedra in the ternary \( \text{P} \) and \( \text{TiNiSi} \) type structures. There it is sometimes called the tetrahedral site, because the four P neighbors form distorted tetrahedra. One Co atom has a coordination of 10 metal and 5 P atoms. The latter form a square pyramid. It corresponds to site a of the large tetrahedra in the ternary \( \text{P} \) and \( \text{TiNiSi} \) type structures. The thermal parameters of the Co atoms correlate with the coordination numbers: large thermal amplitudes are observed for sites with large coordination numbers. This is also the case in related structures as in \( \text{ErCo}_3\text{P}_3 \) and \( \text{Er}_2\text{Ni}_12\text{P}_7 \) (Jeitschko and Jaberg, Z. Anorg. Allg. Chem. (1980) 467, 95) and \( \text{Nd}_2\text{Ni}_12\text{P}_7 \) (Guéritin, Potel, Sergent, J. Less-Common Met. (1981) 78, 177).

Fig. 1. Comparison of the crystal structures of \( \text{LaCo}_3\text{P}_5 \) and \( \text{LaCo}_3\text{P}_5 \). The trigonal prisms of metal atoms (large circles: \( \text{La} \), small circles: \( \text{Co} \) around the \( P \) atoms (filled circles) are emphasized. Atoms connected by thin and thick lines are separated from each other by half a translation period of the projection direction.

Fig. 2. Similarities of the structures of \( \text{YCo}_3\text{P}_3 \), \( \text{LaCo}_3\text{P}_5 \), and \( \text{YNi}_3\text{Si}_3 \) (\( \text{YNi}_3\text{Si}_3 \) type). The trigonal prisms of metal atoms (large and small circles for the rare earth and transition metals respectively) around the metalloid atoms (black dots) are emphasized. Atoms connected by thin and thick lines are separated from each other by half a translation period of the projection direction.

Fig. 1. Crystal structure and near-neighbor coordinations of \( \text{YCo}_3\text{P}_3 \). Atoms connected by thin and thick lines are at \( y = 1/4 \) and \( 3/4 \) respectively. The coordination polyhedra all have mirror planes perpendicular to the projection direction.