

NEW TERNARY PHOSPHIDE $\text{Y}_5\text{Pd}_{19}\text{P}_{12}$ AND IT'S CRYSTAL STRUCTURE*Karychort O. R.*^{1,2}, Zhak O. V.¹, Prots Yu. M.², Grin Yu. M.²¹Ivan Franko National University of Lviv, Kyryla and Mefodiya Str., 6, 79005 Lviv, Ukraine²Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

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A great variety of structure types characterizes the ternary systems *RE-M-P* containing the rare earth (*RE*), the transition metal (*M*) and phosphorus. Nearly all of these systems have representatives of the ThCr_2Si_2 , TiNiSi , $\text{Hf}_2\text{Co}_4\text{P}_3$, and $\text{Zr}_2\text{Fe}_{12}\text{P}_7$ structure types [1], while some of them have only one representative.

The crystal structure of the $\text{Hf}_2\text{Co}_4\text{P}_3$ [2] type has similar atomic arrangements to the ternary phosphides with the [3], $\text{Sc}_5\text{Co}_{19}\text{P}_{12}$ [4], $\text{Nd}_5\text{Cu}_{17.8}\text{P}_{12}$ [5], and $\text{Ce}_5\text{Cu}_{19}\text{P}_{12}$ [6] structure types. The $\text{Ho}_5\text{Ni}_{19}\text{P}_{12}$ type crystallizes in the *P*-62*m* space group and can be obtained from the $\text{Hf}_2\text{Co}_4\text{P}_3$ structure by substituting the Hf atoms by the smaller transition metal atoms in the 3*f* Wyckoff site. A fully ordered distribution of all atoms in the *P*-62*m* space group Wyckoff sites is characteristic of both $\text{Hf}_2\text{Co}_4\text{P}_3$ and $\text{Ho}_5\text{Ni}_{19}\text{P}_{12}$. Worth noting that in some *RE-T-P* systems the formation of $\text{RE}_2\text{T}_4\text{P}_3$ – $\text{RE}_5\text{T}_{19}\text{P}_{12}$ pairs has been observed, notably $\text{Sc}_5\text{Co}_{19}\text{P}_{12}$ – $\text{Sc}_2\text{Co}_4\text{P}_3$, $\text{Sc}_5\text{Ni}_{19}\text{P}_{12}$ – $\text{Sc}_2\text{Ni}_4\text{P}_3$, $\text{Zr}_5\text{Co}_{19}\text{P}_{12}$ – $\text{Zr}_2\text{Co}_4\text{P}_3$, $\text{Hf}_5\text{Co}_{19}\text{P}_{12}$ – $\text{Hf}_2\text{Co}_4\text{P}_3$ and $\text{Gd}_5\text{Co}_{19}\text{P}_{12}$ – $\text{Gd}_2\text{Co}_4\text{P}_3$ [1], suggesting the formation of a series of solid solutions.

For the preparation of the single crystals of the new phosphide, the mixture of the starting components (powders of yttrium, palladium and red phosphorus, all with a declared purity better than 99.99 wt.%, Alfa-Aesar, Johnson Matthey Company) in the stoichiometric ratio $\text{Y}:\text{Pd}:\text{P} = 14:57:29$ was pressed under the pressure of 5 MPa. The sample was sealed in a silica tube filled with Ar under 0.4 bar in an alumina crucible, heated to 1000 °C for 72 h, sintered for 5 days and slowly cooled to 100 °C. From the crushed sample, single crystals of phosphide $\text{Y}_5\text{Pd}_{19}\text{P}_{12}$ were mechanically extracted. Data were collected using a Rigaku AFC7 diffractometer with Saturn 724 + CCD detector (MoK α radiation, $\lambda = 0.71073$ Å). All calculations used to determine and refine the crystal structure were performed using WinCSD software [7].

Crystal structure of the ternary compound $\text{Y}_5\text{Pd}_{19}\text{P}_{12}$ has been refined from the single crystal data: *Z* = 2, $\text{Th}_5\text{Fe}_{19}\text{P}_{12}$ -type structure [8], space group *C2/m*, *a* = 32.4160(6) Å, *b* = 3.9311(6) Å, *c* = 9.7266(15) Å, $\beta = 98.205(5)^\circ$; residuals are $R_F = 0.0304$; $wR_P = 0.0558$.

New palladium arsenide belongs to a large family of compounds with a metal to metalloid ratio of 2:1. Atoms in this structure are placed in two mirror planes and perpendicular to short axis. Phosphorous atoms in this structure have coordination number equal to nine, where six of them are forming trigonal prisms centered by P-atoms.

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