

CRYSTAL STRUCTURE OF $Dy_{5+x}Pd_{19-x}P_{12}$ *Karychort O.*¹, Zhak O.¹, Prots Yu.², Onuk O.¹¹Ivan Franko National University of Lviv, Lviv, Ukraine²Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

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Despite numerous investigations in material science and solid-state chemistry, the search for new compounds and measurements of their properties are still quite important for modern science. Ternary phosphides of rare earth metals and transition metals are quite promising for their physical properties and sustainability under extreme conditions such as high temperatures and/or aggressive surroundings.

The ternary systems $RE-Pd-P$, where RE is a heavy rare earth metal, are characterized by a large variety of structure types. Practically, each system has representatives of $ThCr_2Si_2$ and $TiNiSi$ type structures [1], while some structure types have only one representative e.g. $Ho_5Ni_{19}P_{12}$ was established for $Ho_5Pd_{19}P_{12}$ phase [2].

For a similar stoichiometry, the existence of $Ho_5Ni_{19}P_{12}$ [3], $Sc_5Co_{19}P_{12}$ [4], $Nd_5Cu_{17.8}P_{12}$ [5], and $Ce_5Cu_{19}P_{12}$ [6] structure types, which possess similar atomic arrangements were reported. The main difference between these types is the different distribution of atoms in some sites. These four structure types crystallize in the $P-62m$ space group and are derived from the $Hf_2Co_4P_3$ [7] type of structure as a result of substitution of Hf atoms by smaller atoms of transition metals in the $3f$ Wyckoff site.

For the preparation of the single crystals of the new phosphide, the mixture of the initial components (powders of holmium, palladium, and red phosphorus, all with a stated purity better than 99.99 wt%, Alfa-Aesar, Johnson Matthey Company) in stoichiometric ratio $Dy: Pd: P = 26:41:33$ was pressed into the pellet under the pressure of 5 MPa. The sample was sealed into a silica tube filled with Ar under 0.4 bar in an alumina crucible and heated up to 1000 °C for 72 h, sintered for 5 days and then slowly cooled down to 100 °C. The single crystals of the phosphide $Dy_{5+x}Pd_{19-x}P_{12}$ were mechanically extracted from the crushed sample. Data collection was performed using a Rigaku AFC7 diffractometer equipped with a Saturn 724 + CCD detector (MoK α radiation, $\lambda = 0.71073$ Å). All calculations concerning the crystal structure determination and refinement were performed using the WinCSD software [8].

The new ternary phosphide $Dy_{5+x}Pd_{19-x}P_{12}$ crystal structure has been determined using X-ray single crystal data: space group $P-62m$, refined lattice parameters are $a=1.31333(5)$ nm, $c = 0.40032(2)$ nm; residuals are $R_F = 0.0377$; $wR_F = 0.0382$. The atoms in the structure $Dy_{5+x}Pd_{19-x}P_{12}$ are located on mirror planes at $z = 1/4$ and $z = 3/4$. All phosphorus atoms have trigonal prismatic coordination formed only by the metal atoms, which is typical for the intermetallic compounds of transition metals and phosphorous. Other peculiarities of the $Dy_{5+x}Pd_{19-x}P_{12}$ crystal structure are discussed.

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