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New Phosphides with Transition and Rare-Earth Metals and Their Crystal Structures

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NEW PHOSPHIDES WITH TRANSITION AND RARE-EARTH METALS AND THEIR CRYSTAL STRUCTURES

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The interaction between components in systems M - M' - P (M - Zr, Hf, Nb, Mo, W, Mn, Re; M' - V, Cr, Fe, Co, Ni, Cu), Ln - {Fe, Co, Ni, Cu}-P (Ln-rare-earth metals) and $M - \{Si, B\}-P (M - Cr, Mo, W, Mn, Re, Co, Ni, Cu) have been$ investigated and isotermal sections for 47 ternary systems have been built. 98 new phosphides have been synthesized and the crystal structure for 76 has been determined. The structures of new compounds belong to the known structure types, such as MgCu₂, Mg₆Cu₁₆Si₇, TiNiSi, Zr₂Fe₁₂P₇, $\mathrm{Hf_2Co_4P_3}$, $\mathrm{CeAl_2Ga_2}$, $\mathrm{ZrFe_4Si_2}$, $\mathrm{Nb_4CoSi}$, $\mathrm{Mo_5SiB_2}$, $\mathrm{MgZn_2}$ HfCuSi2. The structures of several phosphides represent the new types: Nb_2P , $\alpha-Ni_3P_3$, $Zr_2Ni_{1-x}P$, $Tb_{1-x}NiP$, $SmNi_4P_2$, Nd₃Ni₇P₅, Ni₃,36^{Si}1,76^P6, Mo₂Ni₆P₃, Re₀,6^{Ni}0,4^P The obtained experimental data allowed us to make the following conclusions:

- 1. The atomic substitution of iron triad metals by phosphorus during the solid solution formations in M-M'-P systems was found for the first time.
- 2. Phosphides with 0-0,25 at part P content belong to the structure types, which are usual for intermetallides. The P atoms are cubooktahedr- or icosahedr-coordinated. Both phosphorus and metal atoms occupy the same sites.
- 3. As to phosphides with higher content of P, their phosphorus atoms have trigonal-prismatic or Archimed-cubic coordination.
- 4. New structure types are compared with the known ones.