ScIrP with ZrNiAl-type Structure

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The phosphide ScIrP was synthesized from the elements in a bismuth flux and characterized by powder and single-crystal X-ray diffraction: ZrNiAl type, $P\bar{6}2m$, Z = 3, a = 637.2(3), c = 389.2(2) pm, $wR2$ = 0.0280, 250 F^2 values, 15 variables. The two crystallographically independent phosphorus sites have tricapped trigonal-prismatic metal coordination $P1Ir_3Sc_6$ and $P2Ir_6Sc_3$. The shortest interatomic distances occur for Ir–P (244 – 251 pm) within the 3D [IrP] network in which the scandium atoms fill cavities of coordination number 15 (4 Sc + 6 Ir + 5 P).

Key words: Phosphide, Scandium, Crystal Structure