

$\text{Zr}_2\text{Fe}_{12}\text{P}_7$	$hP21$	$(174) P-6 - k^3j^3fca$
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**$\text{Zr}_2\text{Fe}_{12}\text{P}_7$**  [1];  $\text{Mg}_{2.5}\text{Ni}_{11.5}\text{P}_7$  [3];  $\text{Pb}_7\text{Cl}_2\text{F}_{12}$  ordered [2]  
 Structural features: Infinite columns of base-linked  $\text{P}(\text{Zr}_2\text{Fe}_4)\text{Fe}_3$  and  $\text{PFe}_6\text{Fe}_3$  tricapped trigonal prisms share atoms to form a 3D-framework with propeller-like columns. Derivative of  $\text{Zr}_2\text{Rh}_{12}\text{P}_7$  with an ordered atom arrangement along the c-axis. See Fig. IV.89.

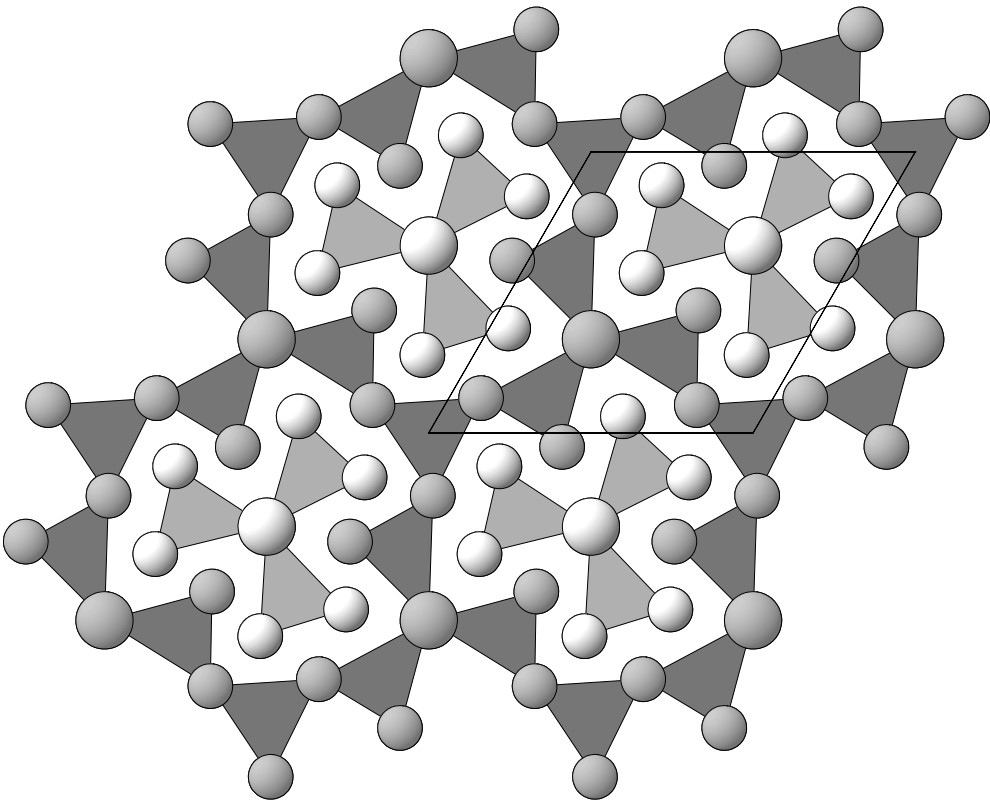


Fig. IV.89.  $\text{Zr}_2\text{Fe}_{12}\text{P}_7$

Arrangement of  $\text{P}(\text{Zr}_2\text{Fe}_4)$  and  $\text{PFe}_6$  trigonal prisms (Zr atoms large, Fe atoms small) viewed along [001]. Light and dark prisms are shifted by  $c/2$ .

Ganglberger E. (1968) [1]

$\text{Fe}_{12}\text{P}_7\text{Zr}_2$

$a = 0.90002$ ,  $c = 0.3592$  nm,  $c/a = 0.399$ ,  $V = 0.2520$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Fe1	$3k$	$m..$	0.0495	0.4359	$\frac{1}{2}$		cuboctahedron $\text{P}_4\text{Fe}_5\text{Zr}_3$
Fe2	$3k$	$m..$	0.2232	0.124	$\frac{1}{2}$		14-vertex polyhedron $\text{P}_5\text{Fe}_9$
P3	$3k$	$m..$	0.2889	0.4096	$\frac{1}{2}$		tricapped trigonal prism $\text{Fe}_7\text{Zr}_2$
Fe4	$3j$	$m..$	0.1189	0.2772	0		cuboctahedron $\text{P}_4\text{Fe}_7\text{Zr}$
P5	$3j$	$m..$	0.4163	0.1204	0		tricapped trigonal prism $\text{Fe}_7\text{Zr}_2$
Fe6	$3j$	$m..$	0.4309	0.3719	0		cuboctahedron $\text{P}_4\text{Fe}_5\text{Zr}_3$
Zr7	$1f$	$-6..$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$		23-vertex polyhedron $\text{P}_9\text{Fe}_{12}\text{Zr}_2$
Zr8	$1c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	0		23-vertex polyhedron $\text{P}_9\text{Fe}_{12}\text{Zr}_2$
P9	$1a$	$-6..$	0	0	0		tricapped trigonal prism $\text{Fe}_9$

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Transformation from published data:  $-y, -x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays,  $R = 0.067$

Remarks: For  $\text{Mg}_{2.5}\text{Ni}_{11.5}\text{P}_7$  [3] partial substitution by Mg on one of the Ni sites is reported. In table I of [2] ( $\text{Pb}_7\text{Cl}_2\text{F}_{12}$ ) the  $y$ -coordinate of site F(3) is misprinted as 0.4600 instead of 0.0460 (checked on interatomic distances).

References: [1] Ganglberger E. (1968), *Monatsh. Chem.* 99, 557-565. [2] Aurivillius B. (1976), *Chem. Scr.* 10, 206-209. [3] Mewis A. (1980), *Z. Naturforsch. B* 35, 620-625.