$Zr_6Ni_{20}P_{13}$	*hP*39	(174) *P*-6 – k^6j^6fca

$Zr_6Ni_{20}P_{13}$ [1]; $U_6Rh_{20}P_{13}$ [2]; $Y_6Ni_{20}P_{13}$ [3]
Structural features: Infinite columns of base-linked $P(Zr_4Ni_2)Ni_3$, $P(Zr_2Ni_4)Ni_3$ and PNi_6Ni_3 tricapped trigonal prisms share atoms to form a 3D-framework with AlB_2-type columns (7 prisms in the dented triangular cross-section). Derivative of $Ho_6Ni_{20}P_{13}$.

Guérin R. et al. (1984) [1]
$Ni_{20}P_{13}Zr_6$
a = 1.2485, c = 0.3622 nm, c/a = 0.290, V = 0.4889 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ni1	3*k*	*m*..	0.0183	0.586	$^1/_2$		cuboctahedron $P_4Ni_4Zr_4$
Ni2	3*k*	*m*..	0.0789	0.1623	$^1/_2$		14-vertex polyhedron P_5Ni_9
Zr3	3*k*	*m*..	0.1888	0.4732	$^1/_2$		22-vertex polyhedron $P_8Ni_{10}Zr_4$
P4	3*k*	*m*..	0.289	0.2312	$^1/_2$		tricapped trigonal prism Ni_7Zr_2
Ni5	3*k*	*m*..	0.3238	0.0716	$^1/_2$		cuboctahedron $P_4Ni_5Zr_3$
P6	3*k*	*m*..	0.5279	0.1406	$^1/_2$		tricapped trigonal prism Ni_5Zr_4
P7	3*j*	*m*..	0.0483	0.2834	0		tricapped trigonal prism Ni_7Zr_2
P8	3*j*	*m*..	0.139	0.613	0		tricapped trigonal prism Ni_5Zr_4
Ni9	3*j*	*m*..	0.2012	0.1068	0		cuboctahedron P_4Ni_7Zr
Ni10	3*j*	*m*..	0.2473	0.3256	0		cuboctahedron $P_4Ni_5Zr_3$
Ni11	3*j*	*m*..	0.4414	0.0213	0		cuboctahedron $P_4Ni_4Zr_4$
Zr12	3*j*	*m*..	0.4739	0.2799	0		22-vertex polyhedron $P_8Ni_{10}Zr_4$
Ni13	1*f*	-6..	$^2/_3$	$^1/_3$	$^1/_2$		tricapped trigonal prism P_3Zr_6
Ni14	1*c*	-6..	$^1/_3$	$^2/_3$	0		tricapped trigonal prism P_3Zr_6
P15	1*a*	-6..	0	0	0		tricapped trigonal prism Ni_9

Transformation from published data: *y*,*x*,*z*
Experimental: single crystal, diffractometer, X-rays, wR = 0.031

Remarks: The *a*-parameter is given as 1.2482 nm on page 1266 but as 1.2485 nm on page 1259. The same data are also reported in [4]. In table III of [1] the Wyckoff position of former Ni(VIII) is misprinted as 1*c* instead of 1*e*. In the abstract of [2] the Hermann-Mauguin symbol for the space group is misprinted as *P*6 instead of *P*-6. In [3] the Wyckoff position of site Ni(2) is misprinted as 1*d* instead of 1*f*.

References: [1] Guérin R., Ghadraoui E.H., Pivan J., Padiou J., Sergent M. (1984), Mater. Res. Bull. 19, 1257-1270. [2] Ghetta V., Chaudouet P., Madar R., Sénateur J.P., Lambert Andron B. (1987), Mater. Res. Bull. 22, 483-488. [3] Chykhrii S.I., Aksel'rud L.G., Oryshchyn S.V., Kuz'ma Y.B. (1985), Dopov. Akad. Nauk Ukr. RSR, Ser. B 1985(11), 57-60. [4] Madar R., Chaudouet P., Dhahri E., Sénateur J.P., Fruchart R., Lambert B. (1985), J. Solid State Chem. 56, 335-342.