

ZrNiAl [2]; CeNiAl [5]; HoMnGa [3]; HoNiAl [5]; LiPrGe [7]; NbFeB [8]; YbPdAs [4]; ZrRuSi [6]

Structural features: Infinite columns of base-linked NiZr_6Al_3 and NiAl_6Zr_3 tricapped trigonal prisms share atoms to form a 3D-framework (a framework of base- and edge-linked NiZr_6 prisms with single columns of base-linked NiAl_6 trigonal prisms shifted by $c/2$ in channels). Ordering variant of Fe_2P . No B-B contact in isotypic borides. See Fig. IV.3.

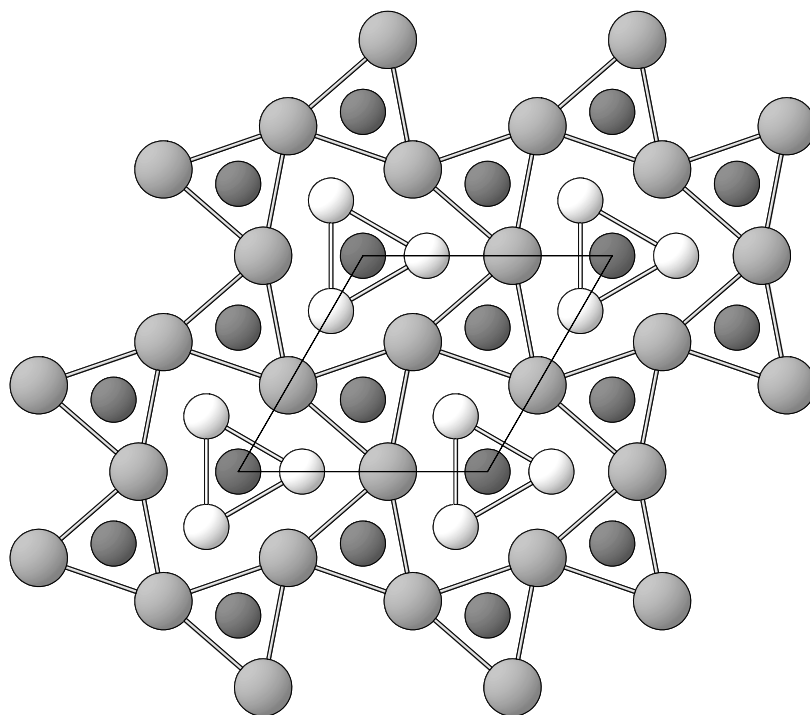


Fig. IV.3. **ZrNiAl**

Arrangement of Zr_6 (Zr atoms large) and Al_6 (Al atoms light) trigonal prisms centered by Ni atoms (dark) viewed along [001].

Zumdick M.F. et al. (1999) [1]

AlNiZr

$a = 0.6906$, $c = 0.3464$ nm, $c/a = 0.502$, $V = 0.1431$ nm³, $Z = 3$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Al1	3g	$m2m$	0.2505	0	$\frac{1}{2}$		14-vertex Frank-Kasper $\text{Ni}_4\text{Zr}_6\text{Al}_4$
Zr2	3f	$m2m$	0.5925	0	0		7-capped pentagonal prism $\text{Ni}_5\text{Al}_6\text{Zr}_6$
Ni3	2d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism Al_3Zr_6
Ni4	1a	-62m	0	0	0		tricapped trigonal prism Al_6Zr_3

Transformation from published data: origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.026$

Remarks: In [8] (NbFeB) the atom coordinates of the second B site are misprinted as $0\ 0\ \frac{1}{2}$ instead of $0\ 0\ 0$; the Wyckoff positions correspond to sites with $z + \frac{1}{2}$. Al and Ga generally prefer the (tetrahedral) site in Wyckoff position 3g, but Si, Ge and B the prism-centering sites in Wyckoff positions 2d and 1a.

References: [1] Zumdick M.F., Hoffmann R.D., Pöttgen R. (1999), Z. Naturforsch. B 54, 45-53. [2] Krypyakevich P.I., Markiv V.Y., Melnyk Y.V. (1967), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1967, 750-753. [3] Brabers J.H.V.J., De Boer F.R., Buschow K.H.J. (1992), J. Alloys Compd. 179, 227-233. [4] Johrendt D., Mewis A. (1992), J. Alloys Compd. 183, 210-223. [5] Dwight A.E., Mueller M.H., Conner R.A. Jr., Downey J.W., Knott H. (1968), Trans. Metall. Soc. AIME 242, 2075-2080. [6] Johnson V., Jeitschko W. (1972), J. Solid State Chem. 4, 123-130. [7] Grund I., Zwiener G., Schuster H.U. (1986), Z. Anorg. Allg. Chem. 535, 7-12. [8] Kuz'ma Y.B. (1967), Dopov. Akad. Nauk Ukr. RSR, Ser. A 1967, 939-940.