$Nd_{42}Ni_{21.67}Si_{31}$	*hP*194	(176) $P6_3/m - h^{31}eca$

$Nd_{42}Ni_{22-x}Si_{31}$ [1]
Structural features: $SiNd_6Ni_3$, $SiNd_6(NdNi_2)$ and $SiNd_6(Nd_2Ni)$ tricapped trigonal prisms (non-parallel prism axes) share atoms to form a 3D-framework with AlB_2-type (LiBaNi) columns (9 prisms in the triangular cross-section); additional Ni in channels of hexagonal cross-section parallel to [001].

Prots' Y.M., Jeitschko W. (1998) [1]
$Nd_{42}Ni_{21.66}Si_{31}$
$a = 3.399$, $c = 0.41783$ nm, $c/a = 0.123$, $V = 4.1805$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Si1	6*h*	*m*..	0.0178	0.2369	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Ni2	6*h*	*m*..	0.02263	0.31055	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Nd3	6*h*	*m*..	0.02878	0.09313	$^1/_4$		
Nd4	6*h*	*m*..	0.03241	0.47939	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Si5	6*h*	*m*..	0.0387	0.5785	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Si6	6*h*	*m*..	0.0959	0.3765	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Ni7	6*h*	*m*..	0.09907	0.44894	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Nd8	6*h*	*m*..	0.11017	0.23011	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Si9	6*h*	*m*..	0.1556	0.0618	$^1/_4$		tricapped trigonal prism $NiNd_8$
Nd10	6*h*	*m*..	0.16632	0.16275	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Nd11	6*h*	*m*..	0.17239	0.54461	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Nd12	6*h*	*m*..	0.18739	0.36719	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Ni13	6*h*	*m*..	0.22377	0.05526	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Nd14	6*h*	*m*..	0.24207	0.29203	$^1/_4$		pseudo Frank-Kasper $Ni_6Si_6Nd_8$
Nd15	6*h*	*m*..	0.26183	0.50259	$^1/_4$		7-capped pentagonal prism $Ni_3Si_5Nd_9$
Ni16	6*h*	*m*..	0.27254	0.59358	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Si17	6*h*	*m*..	0.2965	0.1225	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Nd18	6*h*	*m*..	0.3043	0.22426	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Nd19	6*h*	*m*..	0.31789	0.4293	$^1/_4$		pseudo Frank-Kasper $Ni_6Si_6Nd_8$
Si20	6*h*	*m*..	0.3587	0.0448	$^1/_4$		tricapped trigonal prism Ni_3Nd_6
Si21	6*h*	*m*..	0.3608	0.5412	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Ni22	6*h*	*m*..	0.36313	0.11507	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Nd23	6*h*	*m*..	0.3806	0.35373	$^1/_4$		pseudo Frank-Kasper $Ni_6Si_6Nd_8$
Ni24	6*h*	*m*..	0.42497	0.04008	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Si25	6*h*	*m*..	0.4342	0.1822	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Nd26	6*h*	*m*..	0.44385	0.28621	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Ni27	6*h*	*m*..	0.50402	0.1799	$^1/_4$		tricapped trigonal prism Si_3Nd_6
Nd28	6*h*	*m*..	0.52186	0.10771	$^1/_4$		7-capped pentagonal prism $Ni_2Si_5Nd_{10}$
Si29	6*h*	*m*..	0.5557	0.3142	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Nd30	6*h*	*m*..	0.60607	0.25935	$^1/_4$		pseudo Frank-Kasper $Si_6Ni_5Nd_9$
Si31	6*h*	*m*..	0.6125	0.0997	$^1/_4$		tricapped trigonal prism Ni_2Nd_7
Ni32	4*e*	3..	0	0	0.086	0.207	
Si33	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		tricapped trigonal prism Ni_3Nd_6
Ni34	2*a*	-6..	0	0	$^1/_4$	0.25	

Experimental: single crystal, diffractometer, X-rays, R = 0.030

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Prots' Y.M., Jeitschko W. (1998), J. Solid State Chem. 137, 302-310.