$Sm_{15}Ni_{52}Ga_{44}$	*hP*111	(187) *P*-6*m*2 – $o^3n^6k^3j^3i^3h^4g^3a$

$Sm_{15}Ni_{52}Ga_{44}$ [2]
Structural features: $Sm(Ni,Ga)_{18}$ double hexagonal antiprisms with no, one or two capping Ni or Ga, share atoms to form a dense 3D-framework.

Wasylechko L.O. et al. (1992) [1]
$Ga_{44}Ni_{52}Sm_{15}$
a = 0.8771, c = 2.5061 nm, c/a = 2.857, V = 1.6697 nm^3, Z = 1

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ga1	12*o*	1	0.00233	0.28567	0.0837		icosahedron Ga_8NiSm_3
Ni2	12*o*	1	0.02333	0.36567	0.2504		pseudo Frank-Kasper $Ni_7Ga_3Sm_3$
Ni3	12*o*	1	0.03133	0.37167	0.4168		pseudo Frank-Kasper $Ni_8Ga_2Sm_3$
Ni4	6*n*	.*m*.	0.15833	0.84167	0.343		pseudo Frank-Kasper Ni_8Sm_3
Ga5	6*n*	.*m*.	0.17233	0.82767	0.154		pseudo Frank-Kasper Ga_7Ni_3Sm
Ga6	6*n*	.*m*.	0.50333	0.49667	0.1516		icosahedron $Ga_6Ni_3Sm_3$
Ni7	6*n*	.*m*.	0.52533	0.47467	0.329		pseudo Frank-Kasper Ni_8Sm_3
Ga8	6*n*	.*m*.	0.83333	0.16667	0.1729		icosahedron $Ga_7Ni_2Sm_3$
Ni9	6*n*	.*m*.	0.84033	0.15967	0.327		cuboctahedron Ni_8Sm_4
Ni10	3*k*	*mm*2	0.16333	0.83667	$^1/_2$		icosahedron $Ga_4Ni_6Sm_2$
Ga11	3*k*	*mm*2	0.48333	0.51667	$^1/_2$		10-vertex polyhedron Ni_8Ga_2
Ga12	3*k*	*mm*2	0.83533	0.16467	$^1/_2$		icosahedron $Ni_6Ga_2Sm_4$
Ga13	3*j*	*mm*2	0.19133	0.80867	0		pseudo Frank-Kasper $Ni_2Ga_6Sm_3$
Ni14	3*j*	*mm*2	0.49333	0.50667	0		cuboctahedron Ga_8Sm_4
Ga15	3*j*	*mm*2	0.81833	0.18167	0		pseudo Frank-Kasper $Ni_2Ga_6Sm_3$
Sm16	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.079		pseudo Frank-Kasper $Ga_{15}Ni_3Sm_2$
Sm17	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.241		sixcapped hexagonal prism $Ni_{12}Ga_6$
Sm18	2*i*	3*m*.	$^2/_3$	$^1/_3$	0.414		sixcapped hexagonal prism $Ni_{12}Ga_6$
Sm19	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.0835		pseudo Frank-Kasper $Ga_{15}Ni_4$
Ni20	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.204		14-vertex Frank-Kasper $Ga_6Ni_6Sm_2$
Sm21	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.335		pseudo Frank-Kasper Ni_{20}
Ni22	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.453		14-vertex Frank-Kasper $Ni_{10}Ga_3Sm$
Ga23	2*g*	3*m*.	0	0	0.137		14-vertex Frank-Kasper $Ga_{12}Sm_2$
Sm24	2*g*	3*m*.	0	0	0.2549		pseudo Frank-Kasper Ga_7Ni_{12}
Sm25	2*g*	3*m*.	0	0	0.4227		pseudo Frank-Kasper $Ni_{15}Ga_3Sm_2$
Sm26	1*a*	-6*m*2	0	0	0		pseudo Frank-Kasper Ga_{20}

Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ 0
Experimental: single crystal, diffractometer, X-rays, R = 0.079

Remarks: The same data are reported in [2]. In table 1 of [1] the *y*-coordinate of former Ga4 is misprinted as 0.710 instead of 0.170 (see [2]; agreement with Wyckoff position 6*n*).

References: [1] Wasylechko L.O., Sichewich O.M., Grin Y.N. (1992), J. Alloys Compd. 185, 19-24. [2] Grin Y.N., Sichewich O.M., Wasylechko L.O. (1991), Int. Conf. Solid Compd. Trans. El., 10th, Münster 1991, Coll. Abstr. P-169.