Ba_2NiSi_3	*hP*18	(189) *P*-62*m* – kgf^{2}ca

Ba_2NiSi_3 [1]
Structural features: Si_3 triangles alternate with Ni atoms to form infinite $NiSi_3$ chains (infinite columns of base-linked $NiSi_6$ trigonal prisms).

Goodey J. et al. (2000) [1]
Ba_2NiSi_3
a = 1.1392, c = 0.3938 nm, c/a = 0.346, V = 0.4426 nm^3, Z = 3

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
Si1	6*k*	*m*..	0.3161	0.5354	$^1/_2$		4-vertex polyhedron Ni_2Si_2
Si2	3*g*	*m*2*m*	0.1244	0	$^1/_2$		4-vertex polyhedron Ni_2Si_2
Ba3	3*f*	*m*2*m*	0.3819	0	0		pseudo Frank-Kasper $Si_{10}Ni_3Ba_5$
Ba4	3*f*	*m*2*m*	0.7128	0	0		16-vertex Frank-Kasper $Ni_3Si_8Ba_5$
Ni5	2*c*	-6..	$^1/_3$	$^2/_3$	0		trigonal prism Si_6
Ni6	1*a*	-62*m*	0	0	0		trigonal prism Si_6

Transformation from published data: -*x*,-*y*,-*z*
Experimental: single crystal, diffractometer, X-rays, R = 0.050, T = 298 K

References: [1] Goodey J., Mao J., Guloy A.M. (2000), J. Am. Chem. Soc. 122, 10478-10479.