$SmNiGe_3$ Structure: A3BC_oC20_65_2gh_g_h-001

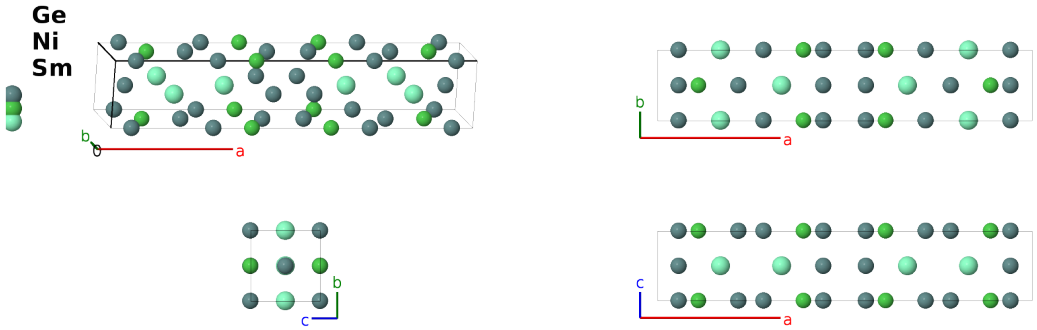
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/Q3JB

https://aflow.org/prototype-encyclopedia/A3BC_oC20_65_2gh_g_h-001



Prototype	Ge_3NiSm
AFLOW prototype label	A3BC_oC20_65_2gh_g_h-001
ICSD	160309
CCDC	1676727
Pearson symbol	oC20
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A3BC_oC20_65_2gh_g_h-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, x_4, x_5$

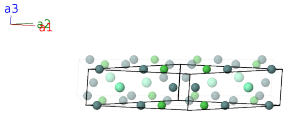
Other compounds with this structure

$CeNiGe_3$, $DyNiGe_3$, $DyNiSi_3$, $ErNiGe_3$, $ErNiSi_3$, $GdNiGe_3$, $HoNiGe_3$, $HoNiSi_3$, $LuNiGe_3$, $NdNiGe_3$, $PrNiGe_3$, $SmNiGe_3$, $TbNiGe_3$, $TmNiGe_3$, $YNiGe_3$, $YbNiGe_3$, $YbNiSi_3$

- (Mun, 2010) give the structure with the long axis of the unit cell along the c-axis. AFLOW rotates this so that it points along the x-axis.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(4g)	Ge I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(4g)	Ge I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}$	(4g)	Ge II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(4g)	Ge II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}}$	(4g)	Ni I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(4g)	Ni I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ge III
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Ge III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sm I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Sm I

References

[1] E. D. Mun, S. L. Bud'ko, H. Ko, G. J. Miller, and P. C. Canfield, *Physical properties and anisotropies of the $RNiGe_3$ series (R = Y, Ce-Nd, Sm, Gd-Lu)*, J. Magn. Magn. Mater. **322**, 3527–3543 (2010), doi:10.1016/j.jmmm.2010.06.057.

Found in

[1] P. Salamakha, M. Konyk, O. Sologub, and O. Bodak, *Ce-Ni-Ge and Nd-Ni-Ge phase diagrams: systematics of rare earth-nickel-germanium compounds*, J. Alloys Compd. **236**, 206–211 (1996), doi:10.1016/0925-8388(95)02081-0.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).