ZrNiAl Structure: ABC_hP9_189_f_bc_g-003

This structure previously used the label(s) `ABC_hP9_189_g_ad_f`. Calls to these addresses will be redirected here.

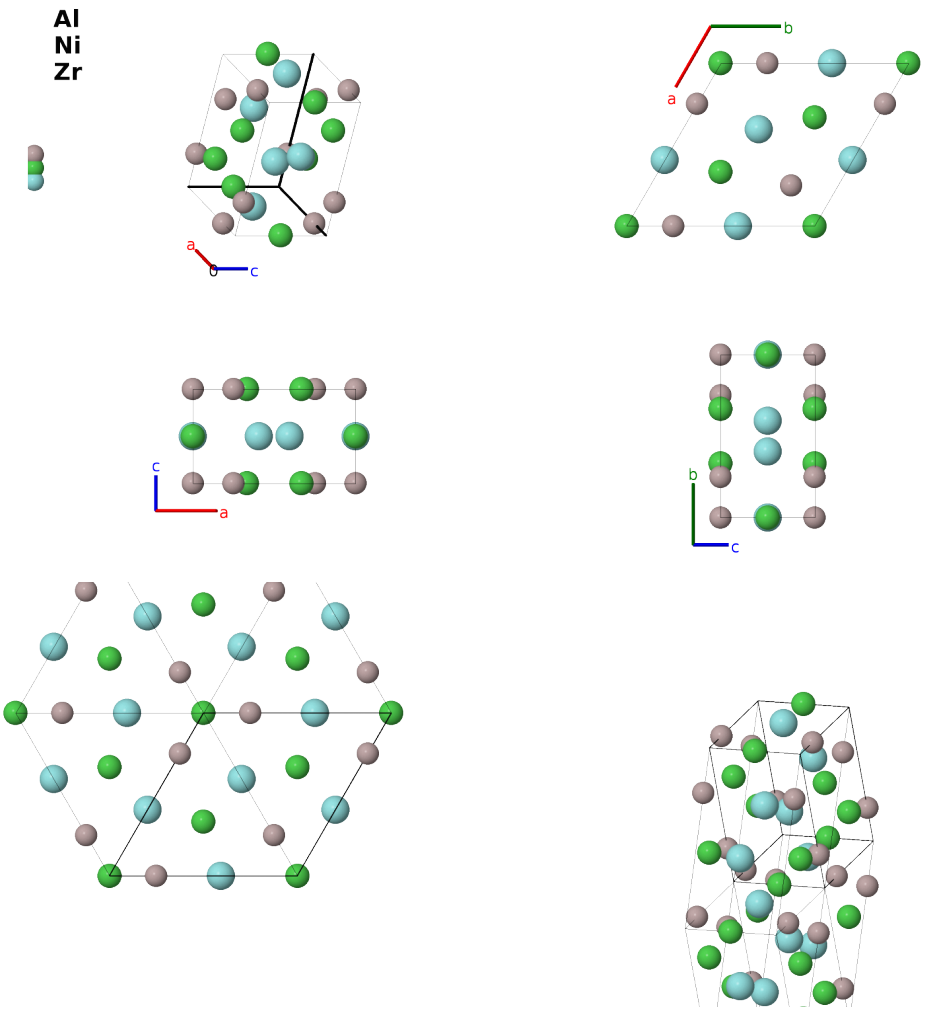
Cite this page as:

- 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/0T4U

https://aflow.org/prototype-encyclopedia/ABC_hP9_189_f_bc_g-003



Prototype	AlNiZr
AFLOW prototype label	ABC_hP9_189_f_bc_g-003
ICSD	152131
CCDC	1668900
Pearson symbol	hP9

Space group number	189
Space group symbol	$P\bar{6}2m$
AFLOW prototype command	`aflow --proto=ABC_hP9_189_f_bc_g-003 --params=`$a, c/a, x_3, x_4$

Other compounds with this structure

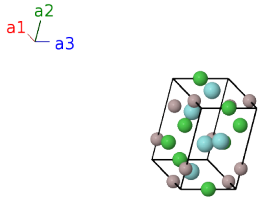
AgAsCa, AgCaAs, AgDyGe, AgDySi, AgErGe, AgErSi, AgGdGe, AgGdSi, AgLuSi, AgMgY, AgMgYSi, AgSiYb, AgSmSi, AgTmSi, AgYSi, AgYbGe, AgYbSi, AlCeCu, AlCeNi, AlCePd, AlCoPu, AlCoTh, AlCoU, AlCuDy, AlCuEr, AlCuGd, AlCuHo, AlCuLu, AlCuNd, AlCuPr, AlCuSm, AlCuTb, AlCuTm, AlCuY, AlCuYb, AlDyNi, AlErNi, AlFeU, AlGdNi, AlHfNi, AlHfPt, AlHoNi, AlIrTh, AlIrU, AlLuNi, AlNdNi, AlNiPr, AlNiPu, AlNiSm, AlNiTb, AlNiTh, AlNiTm, AlNiU, AlNiY, AlNiYb, AlNiZr, AlPdTh, AlPtTh, AlPtU, AlPtZr, AlRhTh, AlRhU, AlRuU, AsCoCr, AuCeIn, AuDyIn, AuErIn, AuGdIn, AuHoIn, AuInLa, AuInLu, AuInNd, AuInPr, AuInSm, AuInTb, AuInTm, AuInY, AuInYb, CaAgAs, CaAgP, CaCdGe, CaCdPb, CaCdSn, CaPbPd, CdCeCu, CdCePd, CdCuDy, CdCuGd, CdCuPr, CdCuSm, CdDyGa, CdErGa, CdGaGd, CdGaNd, CdGaPr, CdGaSm, CdGdPd, CdLaPd, CdPdPr, CdPdSm, CeAgMg, CeAuCd, CeAuIn, CeCuAl, CeCuIn, CeCuMg, CeGaNi, CeInNi, CeInPd, CeInPt, CeInRh, CeIrIn, CeIrSn, CeMgGa, CeMgIn, CeMgTl, CeNiGa, CeNiIn, CeNiZn, CePdAl, CePdIn, CePdMg, CePdSn, CePdTl, CePdZn, CePtCd, CePtIn, CePtMg, CePtSn, CeRhPb, CeRhSn, CeRuSn, CoGaPu, CoGaTh, CoGaU, CoGeTi, CoHfSn, CoNiAs, CoNiP, CoSnTh, CoSnU, CoSnZr, CrCoAs, CrFeAs, CrNiAs, CrNiP, CrPdAs, CrPdP, CrRhAs, CrTiAs, CuDyIn, CuErIn, CuGdIn, CuGeSc, CuHoIn, CuInLa, CuInLu, CuInNd, CuInPr, CuInSm, CuInTb, CuInTm, CuInY, CuScGe, CuScSi, DyAgGe, DyAuIn, DyCuAl, DyCuIn, DyGaMn, DyInNi, DyInPd, DyInPt, DyInRh, DyIrIn, DyLiGe, DyMgIn, DyNiAl, DyNiIn, DyNiSn, DyNiZn, DyPdZn, DyPtIn, DyPtMg, DyPtSn, DyRhBi, DyRhSn, ErAgGe, ErAgPb, ErAgSn, ErAuIn, ErCuAl, ErCuIn, ErInNi, ErInPd, ErInPt, ErInRh, ErIrIn, ErIrSn, ErLiGe, ErNiAl, ErNiIn, ErNiZn, ErPdIn, ErPdSn, ErPdZn, ErPtIn, ErPtSn, ErRhIn, ErRhSn, FeCoAs, FeCrAs, FeGaU, FeGeHf, FeNbB, FeNiAs, FeNiP, FeRhAs, FeRhP, FeTaB, FeTiAs, GaGdMn, GaHfNi, GaHfPt, GaHoMn, GaIrTh, GaIrU, GaMnTb, GaNiPu, GaNiTh, GaNiU, GaNiZr, GaPdSc, GaPdU, GaPtTh, GaPtU, GaPtZr, GaPuRh, GaRhTh, GaRhU, GaRuU, GdAgGe, GdAuMg, GdCuAl, GdCuIn, GdCuMg, GdInNi, GdInPd, GdInPt, GdInRh, GdIrIn, GdMgGa, GdMgIn, GdNiAl, GdNiIn, GdNiSn, GdNiZn, GdPdAl, GdPdCd, GdPdIn, GdPdMg, GdPdTl, GdPdZn, GdPtMg, GdPtPb, GdPtSn, GdRhSn, GeHfMn, GeHfOs, GeHfRh, GeHfRu, GeMnNb, GeMnRh, GeMnSc, GeMnTa, GeOsZr, HfCoSn, HfFeGe, HfIrSn, HfMoP, HfNiAl, HfNiGa, HfOsAs, HfOsP, HfOsSi, HfReSi, HfRhSn, HfRuAs, HfRuP, HfRuSi, HgPdSm, HoAgGe, HoAuIn, HoAuMg, HoCuAl, HoCuIn, HoInNi, HoInPd, HoIrIn, HoIrSn, HoLiGe, HoMgIn, HoNiAl, HoNiIn, HoPdIn, HoPdSn, HoPdZn, HoPtIn, HoPtMg, HoPtSn, HoRhIn, HoRhSn, InLaNi, InLaPd, InLaPt, InLaRh, InLuPt, InNdNi, InNdPd, InNdPt, InNdRh, InNiPr, InNiSm, InNiTb, InNiTh, InNiTm, InNiY, InPdPr, InPdSm, InPdTb, InPdTh, InPdTm, InPdU, InPdY, InPdYb, InPtTh, InPtTm, InPtU, InPtY, InRhU, InRhY, IrGaU, IrLuSn, IrNpSn, IrSnTm, IrSnU, IrSnYb, IrSnZr, LaAuCd, LaAuMg, LaMgGa, LaMgTl, LaNiIn, LaNiZn, LaPdIn, LaPdSn, LaPdTl, LaPtSn, LaRhPb, LaRhSn, LiGdGe, LiYGe, LiYSi, LuAgPb, LuAgSn, LuCuAl, LuInNi, LuNiAl, LuNiPb, LuPdSn, LuPdZn, LuPtSn, LuRuGe, MgPbYb, MgPdY, MgSnYb, MnFeAs, MnNiAs, MnNiP, MnPdAs, MnPdGe, MnPdP, MnRhAs, MnRhP, MnRuAs, MnTaSi, MnTiAs, MnTiSi, MoNiP, NaBaBi, NaBaP, NaSrAs, NaSrP, NbCrGe, NbCrSi, NbMnGe, NbMnSi, NbReSi, NdAgMg, NdCuAl, NdCuIn, NdLiGe, NdMgGa, NdNiAl, NdNiIn, NdPdIn, NdPdSn, NdPdTl, NdPdZn, NdPtMg, NdPtSn, NdRhSn, NiCoP, NiGaTh, NiGaU, NiMoP, NiPdAs, NiPdP, NiPdSi, NiPrZn, NiRhP, NiSmZn, NiWP, OsTiP, OsZrAs, OsZrP, PbPdY, PdMnGe, PdPrTl, PdPrZn, PdSmTl, PdSmZn, PdSnTm, PdTbTl, PdTiAs, PdTlYb, PrAuMg, PrCuAl, PrLiGe, PrMgGa, PrNiIn, PrNiSn, PrPdIn, PrPdSn, PrPdZn, PrPtMg, PrPtSn, PrRhIn, PrRhSn, PtGaU, PtScSn, PtSnTb, PtSnTm, PtSnU, PtSnY, PtSnYb, ReSiTa, ReSiZr, RhGaU, RhMnAs, RhSmSn, RhSnTb, RhSnTh, RhSnTm, RhSnU, RhSnY, RhSnYb, RhSnZr, RuSbU, RuSiZr, RuSnU, RuZrAs, RuZrP, RuZrSi, ScAgGe, ScCuGe, ScCuSi, ScFeGe, ScIrP, ScMnGe, ScMnSi, ScNiSn, ScOsGe, ScPdGe, ScPtSn, ScRhGe, ScRuGe, ScRuP, ScRuSi, SmCuAl, SmIrIn, SmLiGe, SmMgGa, SmMgIn, SmMgTl, SmNiAl, SmNiIn, SmPdZn, SmPtIn, SmPtMg, SmPtSn, SmRhIn, TaFeB, TbAgGe, TbAuIn, TbCuAl, TbCuIn, TbIrIn, TbLiGe, TbNiAl, TbNiIn, TbNiZn, TbPdAl, TbPdZn, TbPtIn, TbRhIn, ThCoSn, ThRhAl, TiAsRu, TiCoGe, TiCoSi, TiCrP, TiFeP, TiFeSi, TiPdGe, TiRuP, TmAgGe, TmAgPb, TmAgSi, TmAgSn, TmCuAl, TmMgGa, TmMgIn, TmMnGe, TmNiAl, TmNiIn, TmPdIn, TmPdZn, TmPtIn, TmRhIn, TmRhSn, UAlFe, UAlIr, UAlRh, UAlRu, UCoAl, UCoGa, UCoSn, UGaCo, UGaFe, UGaNi, UGaRu, UIrSn, UNiAl, UNiGa, UNiZn, UPtAl, URhAl, URhSn, URuSn, YAgPb, YCuAl, YCuIn, YCuMg, YMgAl, YMgGa, YMgIn, YMgTl, YMgZn, YPdAl, YPdZn, YPtIn, YPtMg, YbAgGe, YbCdGe, YbCdPb, YbCdSn, YbLiGe, YbMgSn, YbMnGe, YbPdAs, YbPdIn, YbPdSn, YbPtIn, YbPtSn, YbRhSn, ZrIrSn, ZrMoP, ZrNiAl, ZrNiGa, ZrRuAs, ZrRuSi, BSi_2Ni_6

- This a the ternary form of Barringerite (Fe_2P). While (Shved, 2019) placed the nickel atoms on the (1a) and (2d) sites, as in Fe_2P, we have shifted to origin by $\frac{1}{2}c\hat{z}$ to place them on the (1b) and (2c) sites. Otherwise the structures are nearly identical.
- When the atomic species on the (1b) and (2c) sites are different we have the quaternary version of this structure, $Tb_3Mn_3Ga_2Si$.

- (Shved, 2019) found evidence of 6-10% mixing between the Ni-II (2d) and Al (3g) sites.
- (Shved, 2019) has no entry in the ICSD, so we reference the ZrNiAl entry from (Zumdick, 1999).

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ni I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Ni II
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Ni II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	Al I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Zr I

References

[1] O. Shved, L. P. Salamakha, S. Mudry, O. Sologub, P. F. Rogl, and E. Bauer, *Zr-based nickel aluminides: crystal structure and electronic properties*, J. Alloys Compd. p. 153326 (2019), doi:10.1016/j.jallcom.2019.153326. In press.

[2] M. F. Zumdick, R.-D. Hoffmann, and R. Pöttgen, *The Intermetallic Zirconium Compounds ZrNiAl, ZrRhSn, and ZrPtGa - Structural Distortions and Metal-Metal Bonding in Fe_2P Related Compounds*, Z. Naturforsch. B **54**, 45–53 (1999), doi:10.1515/znb-1999-0111.

First cited in

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.