

Pt₃Zn₁₀ Structure:

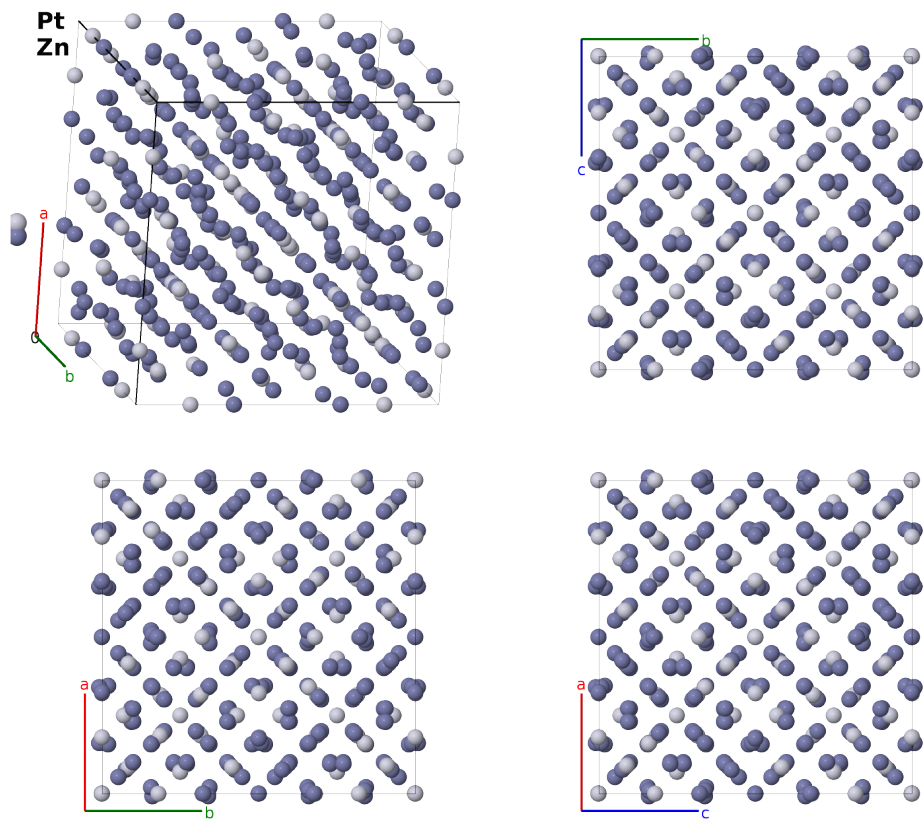
A2B5_cF392_216_4efg_4ef4h-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/V17U>

https://aflow.org/prototype-encyclopedia/A2B5_cF392_216_4efg_4ef4h-001

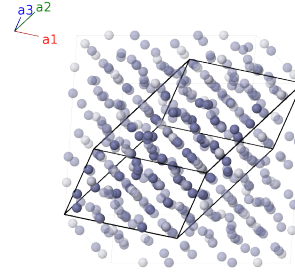


Prototype	Pt ₃ Zn ₁₀
AFLOW prototype label	A2B5_cF392_216_4efg_4ef4h-001
ICSD	105854
CCDC	1663722
Pearson symbol	cF392
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=A2B5_cF392_216_4efg_4ef4h-001</code> <code>--params=$a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}$</code>

- The site occupation in this structure is rather complicated:
 - In any unit cell, only one of the Pt-II/Zn-II sites is occupied.
 - The site we have labeled Pt-II is actually 50% platinum and 50% zinc.
 - The sites we have labeled Zn-II and Zn-V are 8.333% platinum and 91.667% zinc.
 - The Pt-V and Pt-VI sites are 2/3 platinum and 1/3 zinc.
- Accounting for all of this the nominal composition of the structure is approximately $\text{Pt}_3\text{Zn}_{10}$.
- This is an example of an F-cell γ -brass. (Mizutani, 2010)
- (Johansson, 1970) give the Wyckoff positions of the (24h) sites as xyy . The standard representation, used by AFLOW, is xyy , so we have swapped their x and y coordinates for these sites.

Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B}_2$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - 3x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - 3x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B}_4$	$= -3x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16e)	Pt I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16e)	Pt II
$\mathbf{B}_6$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - 3x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(16e)	Pt II
$\mathbf{B}_7$	$= x_2 \mathbf{a}_1 - 3x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16e)	Pt II
$\mathbf{B}_8$	$= -3x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(16e)	Pt II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e)	Pt III
$\mathbf{B}_{10}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(16e)	Pt III
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e)	Pt III
$\mathbf{B}_{12}$	$= -3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(16e)	Pt III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e)	Pt IV
$\mathbf{B}_{14}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(16e)	Pt IV
$\mathbf{B}_{15}$	$= x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e)	Pt IV
$\mathbf{B}_{16}$	$= -3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(16e)	Pt IV
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e)	Zn I
$\mathbf{B}_{18}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(16e)	Zn I

$\mathbf{B}_{19} =$	$x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e)	Zn I
$\mathbf{B}_{20} =$	$-3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(16e)	Zn I
$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e)	Zn II
$\mathbf{B}_{22} =$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(16e)	Zn II
$\mathbf{B}_{23} =$	$x_6 \mathbf{a}_1 - 3x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Zn II
$\mathbf{B}_{24} =$	$-3x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(16e)	Zn II
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Zn III
$\mathbf{B}_{26} =$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - 3x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(16e)	Zn III
$\mathbf{B}_{27} =$	$x_7 \mathbf{a}_1 - 3x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Zn III
$\mathbf{B}_{28} =$	$-3x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(16e)	Zn III
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Zn IV
$\mathbf{B}_{30} =$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - 3x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}}$	(16e)	Zn IV
$\mathbf{B}_{31} =$	$x_8 \mathbf{a}_1 - 3x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Zn IV
$\mathbf{B}_{32} =$	$-3x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + x_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}}$	(16e)	Zn IV
$\mathbf{B}_{33} =$	$-x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}}$	(24f)	Pt V
$\mathbf{B}_{34} =$	$x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}}$	(24f)	Pt V
$\mathbf{B}_{35} =$	$x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{y}}$	(24f)	Pt V
$\mathbf{B}_{36} =$	$-x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{y}}$	(24f)	Pt V
$\mathbf{B}_{37} =$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - x_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{z}}$	(24f)	Pt V
$\mathbf{B}_{38} =$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 + x_9 \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{z}}$	(24f)	Pt V
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}}$	(24f)	Zn V
$\mathbf{B}_{40} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}}$	(24f)	Zn V
$\mathbf{B}_{41} =$	$x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{y}}$	(24f)	Zn V
$\mathbf{B}_{42} =$	$-x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{y}}$	(24f)	Zn V
$\mathbf{B}_{43} =$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{z}}$	(24f)	Zn V
$\mathbf{B}_{44} =$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{z}}$	(24f)	Zn V
$\mathbf{B}_{45} =$	$-\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{46} =$	$x_{11} \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{47} =$	$x_{11} \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + x_{11} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{48} =$	$-\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + x_{11} \mathbf{a}_2 -$ $\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{49} =$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + ax_{11} \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{50} =$	$-\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 +$ $x_{11} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{z}}$	(24g)	Pt VI
$\mathbf{B}_{51} =$	$z_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_2 + (2x_{12} - z_{12}) \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + az_{12} \hat{\mathbf{z}}$	(48h)	Zn VI
$\mathbf{B}_{52} =$	$z_{12} \mathbf{a}_1 + z_{12} \mathbf{a}_2 - (2x_{12} + z_{12}) \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} + az_{12} \hat{\mathbf{z}}$	(48h)	Zn VI
$\mathbf{B}_{53} =$	$(2x_{12} - z_{12}) \mathbf{a}_1 -$ $(2x_{12} + z_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} - az_{12} \hat{\mathbf{z}}$	(48h)	Zn VI
$\mathbf{B}_{54} =$	$-(2x_{12} + z_{12}) \mathbf{a}_1 +$ $(2x_{12} - z_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} - ax_{12} \hat{\mathbf{y}} - az_{12} \hat{\mathbf{z}}$	(48h)	Zn VI
$\mathbf{B}_{55} =$	$(2x_{12} - z_{12}) \mathbf{a}_1 + z_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$az_{12} \hat{\mathbf{x}} + ax_{12} \hat{\mathbf{y}} + ax_{12} \hat{\mathbf{z}}$	(48h)	Zn VI

$$\begin{aligned}
\mathbf{B}_{86} &= \begin{pmatrix} (2x_{14} - z_{14}) \mathbf{a}_1 + z_{14} \mathbf{a}_2 - \\ (2x_{14} + z_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - az_{14} \hat{\mathbf{y}} + ax_{14} \hat{\mathbf{z}} & (48h) & \text{Zn VIII} \\
\mathbf{B}_{87} &= z_{15} \mathbf{a}_1 + z_{15} \mathbf{a}_2 + (2x_{15} - z_{15}) \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} + az_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{88} &= z_{15} \mathbf{a}_1 + z_{15} \mathbf{a}_2 - (2x_{15} + z_{15}) \mathbf{a}_3 = -ax_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + az_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{89} &= \begin{pmatrix} (2x_{15} - z_{15}) \mathbf{a}_1 - \\ (2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - az_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{90} &= \begin{pmatrix} -(2x_{15} + z_{15}) \mathbf{a}_1 + \\ (2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 \end{pmatrix} = ax_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} - az_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{91} &= (2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = az_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{92} &= -(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 = az_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{93} &= z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 - \\ & \quad (2x_{15} + z_{15}) \mathbf{a}_3 = -az_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{94} &= z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 + \\ & \quad (2x_{15} - z_{15}) \mathbf{a}_3 = -az_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{95} &= z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{96} &= z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 = -ax_{15} \hat{\mathbf{x}} + az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{97} &= -(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + \\ & \quad (2x_{15} - z_{15}) \mathbf{a}_3 = ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{98} &= \begin{pmatrix} (2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 - \\ (2x_{15} + z_{15}) \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX}
\end{aligned}$$

References

- [1] A. Johansson and S. Westman, *Determination of the Structure of Cubic Gamma-Pt,Zn; a Phase of Gamma Brass Type with an 18Å Superstructure*, Acta Chem. Scand. **24**, 3471–3479 (1970), doi:10.3891/acta.chem.scand.24-3471.

Found in

- [1] U. Mizutani, *Hume-Rothery Rules for Structurally Complex Alloy Phases* (CRC Press, Boca Raton, London, New York, 2010).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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.