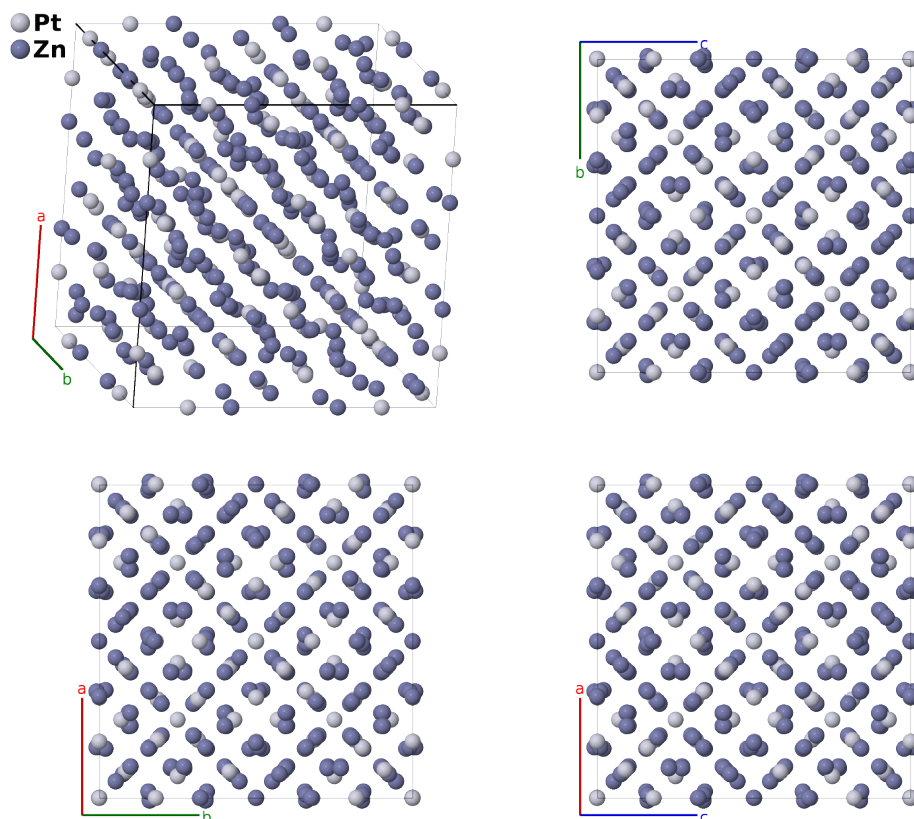


Pt₃Zn₁₀ Structure: A2B5_cF392_216_4efg_4ef4h-001

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<https://aflow.org/p/V17U>

https://aflow.org/p/A2B5_cF392_216_4efg_4ef4h-001



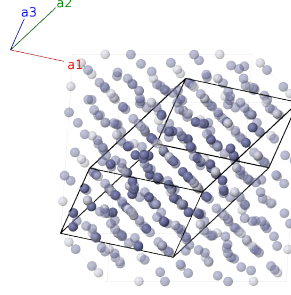
Prototype	Pt ₃ Zn ₁₀
AFLOW prototype label	A2B5_cF392_216_4efg_4ef4h-001
ICSD	105854
Pearson symbol	cF392
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<pre>aflow --proto=A2B5_cF392_216_4efg_4ef4h-001 --params=a, x1, x2, x3, x4, x5, x6, x7, x8, x9, x10, x11, x12, z12, x13, z13, x14, z14, x15, z15</pre>

- 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 xyx , so we have swapped their x and y coordinates for these sites.

Face-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{x} + ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Pt I
\mathbf{B}_2	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - 3x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{x} - ax_1 \hat{y} + ax_1 \hat{z}$	(16e)	Pt I
\mathbf{B}_3	$= x_1 \mathbf{a}_1 - 3x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{x} + ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Pt I
\mathbf{B}_4	$= -3x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{x} - ax_1 \hat{y} - ax_1 \hat{z}$	(16e)	Pt I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} + ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Pt II
\mathbf{B}_6	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - 3x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} - ax_2 \hat{y} + ax_2 \hat{z}$	(16e)	Pt II
\mathbf{B}_7	$= x_2 \mathbf{a}_1 - 3x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{x} + ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Pt II
\mathbf{B}_8	$= -3x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{x} - ax_2 \hat{y} - ax_2 \hat{z}$	(16e)	Pt II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} + ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Pt III
\mathbf{B}_{10}	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - 3x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} - ax_3 \hat{y} + ax_3 \hat{z}$	(16e)	Pt III
\mathbf{B}_{11}	$= x_3 \mathbf{a}_1 - 3x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{x} + ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Pt III
\mathbf{B}_{12}	$= -3x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{x} - ax_3 \hat{y} - ax_3 \hat{z}$	(16e)	Pt III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} + ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Pt IV
\mathbf{B}_{14}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - 3x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} - ax_4 \hat{y} + ax_4 \hat{z}$	(16e)	Pt IV
\mathbf{B}_{15}	$= x_4 \mathbf{a}_1 - 3x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{x} + ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Pt IV
\mathbf{B}_{16}	$= -3x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{x} - ax_4 \hat{y} - ax_4 \hat{z}$	(16e)	Pt IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} + ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Zn I
\mathbf{B}_{18}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 - 3x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} - ax_5 \hat{y} + ax_5 \hat{z}$	(16e)	Zn I
\mathbf{B}_{19}	$= x_5 \mathbf{a}_1 - 3x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{x} + ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Zn I
\mathbf{B}_{20}	$= -3x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{x} - ax_5 \hat{y} - ax_5 \hat{z}$	(16e)	Zn I
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ax_6 \hat{x} + ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Zn II
\mathbf{B}_{22}	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - 3x_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{x} - ax_6 \hat{y} + ax_6 \hat{z}$	(16e)	Zn II

$$\begin{aligned}
\mathbf{B}_{89} &= \begin{matrix} (2x_{15} - z_{15}) \mathbf{a}_1 - \\ (2x_{15} + z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 \end{matrix} &= & -ax_{15} \hat{\mathbf{x}} + ax_{15} \hat{\mathbf{y}} - az_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{90} &= \begin{matrix} -(2x_{15} + z_{15}) \mathbf{a}_1 + \\ (2x_{15} - z_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3 \end{matrix} &= & 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} &= \begin{matrix} z_{15} \mathbf{a}_1 + (2x_{15} - z_{15}) \mathbf{a}_2 - \\ (2x_{15} + z_{15}) \mathbf{a}_3 \end{matrix} &= & -az_{15} \hat{\mathbf{x}} - ax_{15} \hat{\mathbf{y}} + ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{94} &= \begin{matrix} z_{15} \mathbf{a}_1 - (2x_{15} + z_{15}) \mathbf{a}_2 + \\ (2x_{15} - z_{15}) \mathbf{a}_3 \end{matrix} &= & -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} &= \begin{matrix} -(2x_{15} + z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 + \\ (2x_{15} - z_{15}) \mathbf{a}_3 \end{matrix} &= & ax_{15} \hat{\mathbf{x}} - az_{15} \hat{\mathbf{y}} - ax_{15} \hat{\mathbf{z}} & (48h) & \text{Zn IX} \\
\mathbf{B}_{98} &= \begin{matrix} (2x_{15} - z_{15}) \mathbf{a}_1 + z_{15} \mathbf{a}_2 - \\ (2x_{15} + z_{15}) \mathbf{a}_3 \end{matrix} &= & -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.

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