

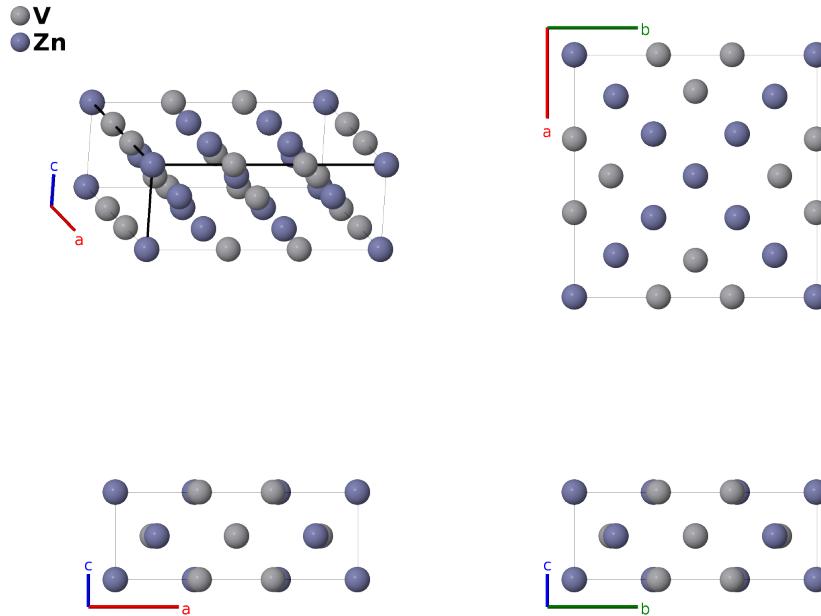
V_4Zn_5 Structure: A4B5_tI18_139_i_ah-001

This structure originally had the label `A4B5_tI18_139_i_ah`. Calls to that address will be redirected here.

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<https://aflow.org/p/84H6>

https://aflow.org/p/A4B5_tI18_139_i_ah-001

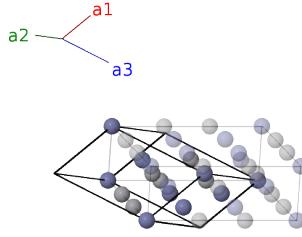


Prototype	V_4Zn_5
AFLOW prototype label	A4B5_tI18_139_i_ah-001
ICSD	106213
Pearson symbol	tI18
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	<code>aflow --proto=A4B5_tI18_139_i_ah-001 --params=a, c/a, x₂, x₃</code>

- This is very similar to the Pt_8Ti structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	=	0	(2a)	Zn I
\mathbf{B}_2	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + 2x_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8h)	Zn II
\mathbf{B}_3	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - 2x_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8h)	Zn II
\mathbf{B}_4	$x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2$	=	$-ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8h)	Zn II
\mathbf{B}_5	$-x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2$	=	$ax_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8h)	Zn II
\mathbf{B}_6	$x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}}$	(8i)	V I
\mathbf{B}_7	$-x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}}$	(8i)	V I
\mathbf{B}_8	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{y}}$	(8i)	V I
\mathbf{B}_9	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{y}}$	(8i)	V I

References

- [1] K. Schubert, H. G. Meissner, A. Raman, and W. Rossteutscher, *Einige Strukturdaten metallischer Phasen (9)*, Naturwissenschaften **51**, 287 (1964), doi:10.1007/BF00625465.

Found in

- [1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.