

V₄Zn₅ Structure:

A4B5_tI18_139_i_ah-001

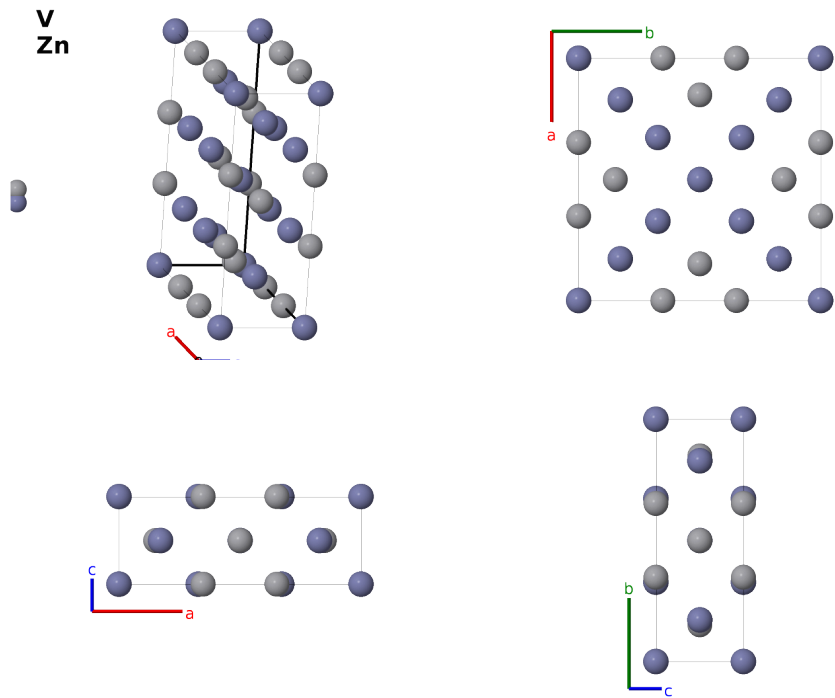
This structure previously used the label(s) **A4B5_tI18_139_i_ah**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/84H6>

https://aflow.org/prototype-encyclopedia/A4B5_tI18_139_i_ah-001

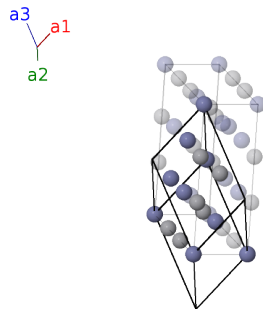


Prototype	V ₄ Zn ₅
AFLOW prototype label	A4B5_tI18_139_i_ah-001
ICSD	106213
CCDC	1664055
Pearson symbol	tI18
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=A4B5_tI18_139_i_ah-001 --params=a, c/a, x₂, x₃</code>

- This is very similar to the Pt₈Ti 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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017