

β -V₃S Structure:

AB3_tP32_133_h_i2j-001

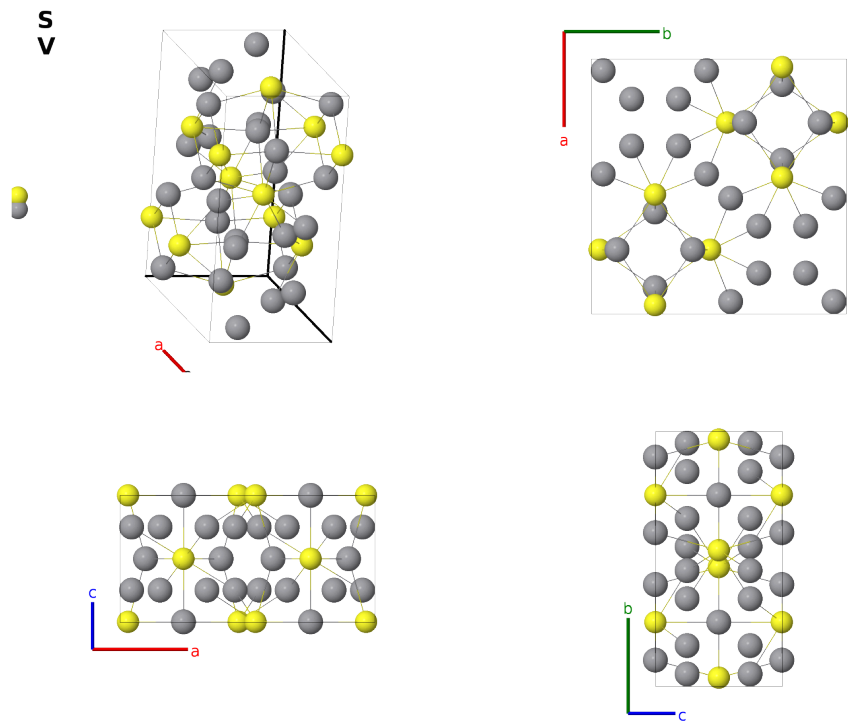
This structure previously used the label(s) **AB3_tP32_133_h_i2j**. Calls to these addresses will be redirected here.

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/2PY4>

https://aflow.org/prototype-encyclopedia/AB3_tP32_133_h_i2j-001



Prototype	SV ₃
AFLOW prototype label	AB3_tP32_133_h_i2j-001
ICSD	26516
CCDC	1601914
Pearson symbol	tP32
Space group number	133
Space group symbol	$P4_2/nbc$
AFLOW prototype command	<code>aflow --proto=AB3_tP32_133_h_i2j-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄</code>

Other compounds with this structure

β -Ta₃P

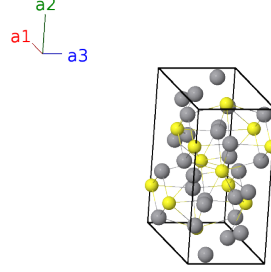
- α -V₃S structure is metastable in this region, and stable above 950°C.
- β -V₃S is stable below 825°C.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	S I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(8h)	S I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	S I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	S I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	S I
$\mathbf{B}_6$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(8h)	S I
$\mathbf{B}_7$	$= \frac{3}{4} \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	S I
$\mathbf{B}_8$	$= \frac{3}{4} \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	S I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{10}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + x_2 \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{14}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8i)	V I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 - x_2 \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8i)	V I
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{18}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{19}$	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{20}$	$= x_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	V II
$\mathbf{B}_{22}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8j)	V II

$$\begin{aligned}
\mathbf{B}_{23} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V II} \\
\mathbf{B}_{24} &= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -ax_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V II} \\
\mathbf{B}_{25} &= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{26} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{27} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{28} &= x_4 \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= ax_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{29} &= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{30} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{31} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V III} \\
\mathbf{B}_{32} &= -x_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}} &(8j) &\text{V III}
\end{aligned}$$

References

- [1] B. Pedersen and F. Grønvold, *The Crystal Structures of α - V_3S and β - V_3S* , Acta Cryst. **12**, 1022–1027 (1959), doi:10.1107/S0365110X59002869.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043