

α -V₃S Structure:

AB3_tI32_121_f_g2i-001

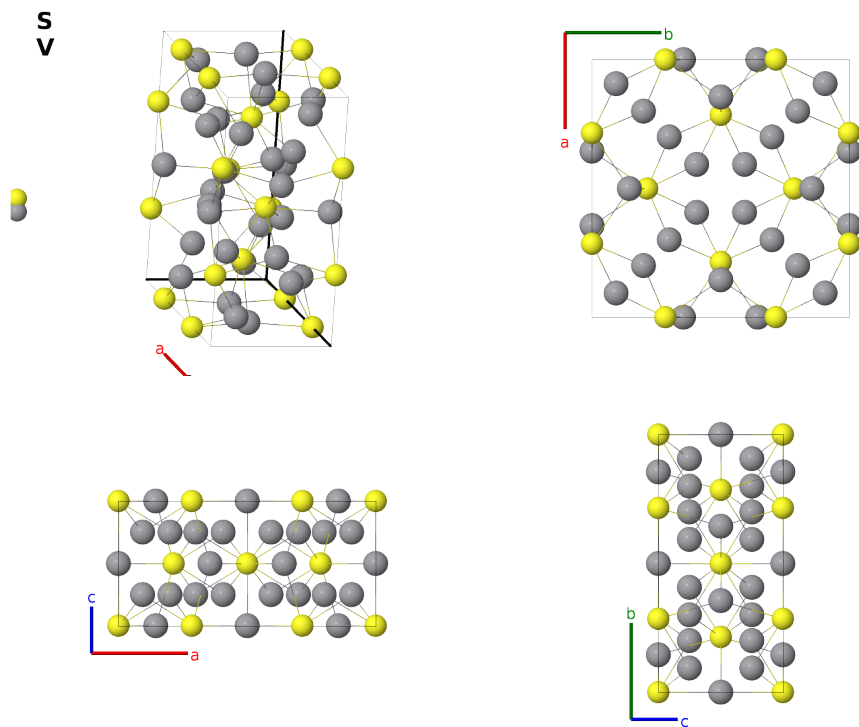
This structure previously used the label(s) **AB3_tI32_121_g_f2i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/QHX2>

https://aflow.org/prototype-encyclopedia/AB3_tI32_121_f_g2i-001



Prototype	SV ₃
AFLOW prototype label	AB3_tI32_121_f_g2i-001
ICSD	26515
CCDC	1601913
Pearson symbol	tI32
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	<code>aflow --proto=AB3_tI32_121_f_g2i-001</code> <code>--params=a, c/a, x₁, x₂, x₃, z₃, x₄, z₄</code>

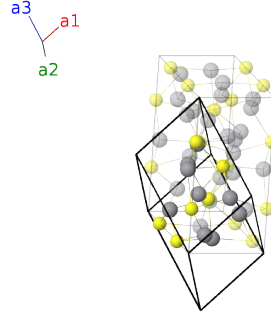
Other compounds with this structure

Mo₃P, Zr₃Ir

- α -V₃S is stable above 950°C, but metastable at 25°C, where this data was taken.
- Below 825°C the system transforms to the β -V₃S structure.
- We have shifted the origin by $1/2$ c $\hat{z}$ from that used by (Pedersen, 1959).

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}}$	(8f)	S I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}}$	(8f)	S I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{y}}$	(8f)	S I
$\mathbf{B}_4$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{y}}$	(8f)	S I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_7$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8g)	V I
$\mathbf{B}_9$	$= (x_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8i)	V II
$\mathbf{B}_{10}$	$= -(x_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8i)	V II
$\mathbf{B}_{11}$	$= -(x_3 + z_3) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8i)	V II
$\mathbf{B}_{12}$	$= (x_3 - z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8i)	V II
$\mathbf{B}_{13}$	$= (x_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + 2x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	V III
$\mathbf{B}_{14}$	$= -(x_4 - z_4) \mathbf{a}_1 - (x_4 - z_4) \mathbf{a}_2 - 2x_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8i)	V III
$\mathbf{B}_{15}$	$= -(x_4 + z_4) \mathbf{a}_1 + (x_4 - z_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	V III
$\mathbf{B}_{16}$	$= (x_4 - z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8i)	V III

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.

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