# $VS_4$ Structure: A4B_mC40_15_4f_f-001

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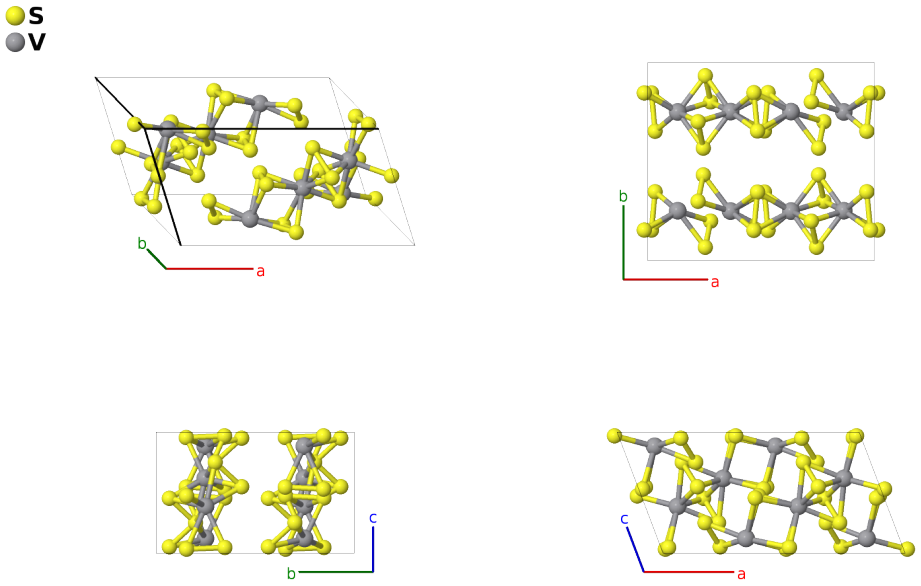
https://aflow.org/p/6M9R

https://aflow.org/p/A4B_mC40_15_4f_f-001

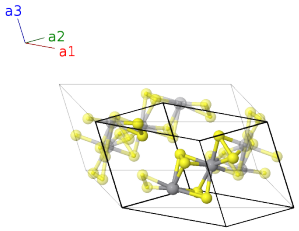



| | |
|---|---|
| **Prototype** | $S_4V$ |
| **AFLOW prototype label** | A4B_mC40_15_4f_f-001 |
| **ICSD** | 16797 |
| **Pearson symbol** | mC40 |
| **Space group number** | 15 |
| **Space group symbol** | $C2/c$ |
| **AFLOW prototype command** | `aflow --proto=A4B_mC40_15_4f_f-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5$ |

- We use the coordinates from (Allmann, 1964) as corrected by (Downs, 2003).
- (Allmann, 1964) give the structure of $VS_4$ in the $I2/c$ setting of space group #15. We used FINDSYM to translate this to the standard $C2/c$ setting.

**Base-centered Monoclinic primitive vectors**

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}
$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $(x_1 - y_1)\,\mathbf{a}_1 + (x_1 + y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_2}$ | = | $-(x_1 + y_1)\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_3}$ | = | $-(x_1 - y_1)\,\mathbf{a}_1 - (x_1 + y_1)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$ | = | $-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_4}$ | = | $(x_1 + y_1)\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$ | = | $\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S I |
| $\mathbf{B_5}$ | = | $(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S II |
| $\mathbf{B_6}$ | = | $-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S II |
| $\mathbf{B_7}$ | = | $-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S II |
| $\mathbf{B_8}$ | = | $(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$ | = | $\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S II |
| $\mathbf{B_9}$ | = | $(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S III |
| $\mathbf{B_{10}}$ | = | $-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S III |
| $\mathbf{B_{11}}$ | = | $-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S III |
| $\mathbf{B_{12}}$ | = | $(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$ | = | $\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S III |
| $\mathbf{B_{13}}$ | = | $(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S IV |
| $\mathbf{B_{14}}$ | = | $-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S IV |
| $\mathbf{B_{15}}$ | = | $-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S IV |
| $\mathbf{B_{16}}$ | = | $(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$ | = | $\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | S IV |
| $\mathbf{B_{17}}$ | = | $(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$ | (8f) | V I |
| $\mathbf{B_{18}}$ | = | $-(x_5 + y_5)\,\mathbf{a}_1 - (x_5 - y_5)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$ | = | $-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$ | (8f) | V I |

$$\mathbf{B_{19}} = -(x_5 - y_5)\ \mathbf{a}_1 - (x_5 + y_5)\ \mathbf{a}_2 - z_5\ \mathbf{a}_3 = -(ax_5 + cz_5 \cos\beta)\ \hat{\mathbf{x}} - by_5\ \hat{\mathbf{y}} - cz_5 \sin\beta\ \hat{\mathbf{z}} \quad (8f) \quad \text{V I}$$

$$\mathbf{B_{20}} = (x_5 + y_5)\ \mathbf{a}_1 + (x_5 - y_5)\ \mathbf{a}_2 + \left(z_5 + \tfrac{1}{2}\right)\ \mathbf{a}_3 = \left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\ \hat{\mathbf{x}} - by_5\ \hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\ \hat{\mathbf{z}} \quad (8f) \quad \text{V I}$$

## References


[1] R. Allmann, I. Baumann, A. Kutoglu, H. Rösch, and E. Hellner, *Die Kristallstruktur des Patronits V($S_2$)$_2$*, Naturwissenschaften **51**, 263–264 (1964), doi:10.1007/BF00638454.


## Found in


[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).