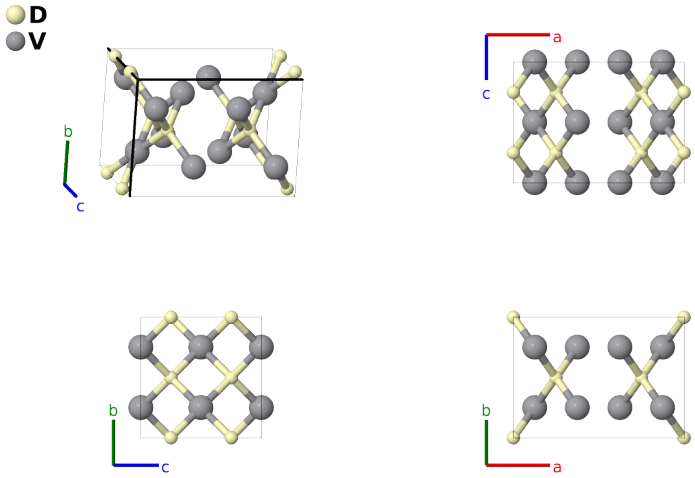
# $\delta$-$V_4D_3$ Structure: A3B4_oP14_49_ej_2q-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/6B3F

https://aflow.org/p/A3B4_oP14_49_ej_2q-001

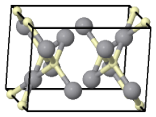



| | |
|---|---|
| **Prototype** | $H_3V_4$ |
| **AFLOW prototype label** | A3B4_oP14_49_ej_2q-001 |
| **ICSD** | 42434 |
| **Pearson symbol** | oP14 |
| **Space group number** | 49 |
| **Space group symbol** | *Pccm* |
| **AFLOW prototype command** | `aflow --proto=A3B4_oP14_49_ej_2q-001 --params=`$a, b/a, c/a, x_2, x_3, y_3, x_4, y_4$ |

- $\delta$-$V_4D_3$ is the only completely ordered structure in the Vanadium-Hydrogen/Deuterium system (Asano, 1973). Even then, the deuterium sites are only 98% occupied.
- The data for this structure was obtained at 88K.
- While (Asano, 1973) placed this in space group *Pcc*2 #27, (Cenzual, 1991) showed that the published coordinates placed the system in space group *Pccm* #49.

**Simple Orthorhombic primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{4}\,\mathbf{a}_3$ | = | $\frac{1}{4}c\,\hat{\mathbf{z}}$ | (2e) | D I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_3$ | = | $\frac{3}{4}c\,\hat{\mathbf{z}}$ | (2e) | D I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4j) | D II |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4j) | D II |
| $\mathbf{B_5}$ | = | $-x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4j) | D II |
| $\mathbf{B_6}$ | = | $x_2\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4j) | D II |
| $\mathbf{B_7}$ | = | $x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$ | = | $ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$ | (4q) | V I |
| $\mathbf{B_8}$ | = | $-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$ | = | $-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$ | (4q) | V I |
| $\mathbf{B_9}$ | = | $-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4q) | V I |
| $\mathbf{B_{10}}$ | = | $x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4q) | V I |
| $\mathbf{B_{11}}$ | = | $x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$ | = | $ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$ | (4q) | V II |
| $\mathbf{B_{12}}$ | = | $-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$ | = | $-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}}$ | (4q) | V II |
| $\mathbf{B_{13}}$ | = | $-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4q) | V II |
| $\mathbf{B_{14}}$ | = | $x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (4q) | V II |

**References**


[1] H. Asano and M. Hirabayashi, *Interstitial superstructures of vanadium deuterides*, phys. stat. sol. (a) **15**, 267–279 (1973), doi:10.1002/pssa.2210150130.


**Found in**


[1] K. Cenzual, L. M. Gelato, M. Penzo, and E. Parthé, *Inorganic structure types with revised space groups. I*, Acta Crystallogr. Sect. B **47**, 433–439 (1991), doi:10.1107/S0108768191000903.