δ-V_4D_3 Structure: A3B4_oP14_49_ej_2q-001

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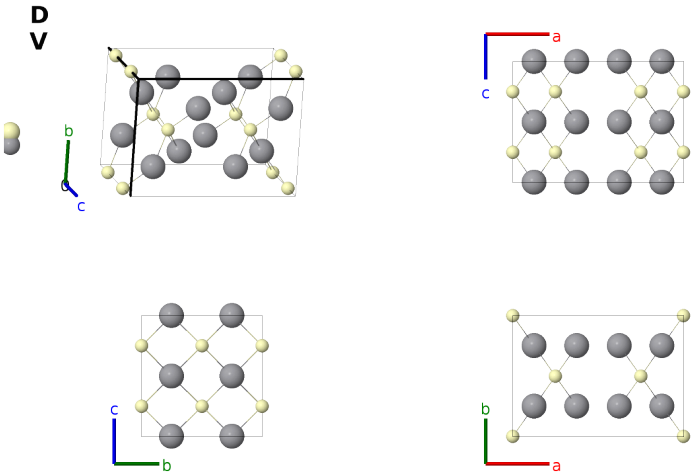
https://aflow.org/prototype-encyclopedia/6B3F

https://aflow.org/prototype-encyclopedia/A3B4_oP14_49_ej_2q-001

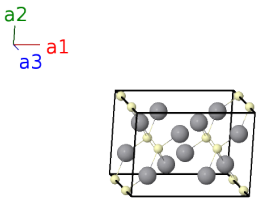


Prototype	H_3V_4
AFLOW prototype label	A3B4_oP14_49_ej_2q-001
ICSD	42434
CCDC	1612100
Pearson symbol	oP14
Space group number	49
Space group symbol	*Pccm*
AFLOW prototype command	`aflow --proto=A3B4_oP14_49_ej_2q-001 --params=`$a, b/a, c/a, x_2, x_3, y_3, x_4, y_4$

- δ-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

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



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

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