$RbVSe_2$ Structure: AB2C_oF64_70_e_h_ab-001

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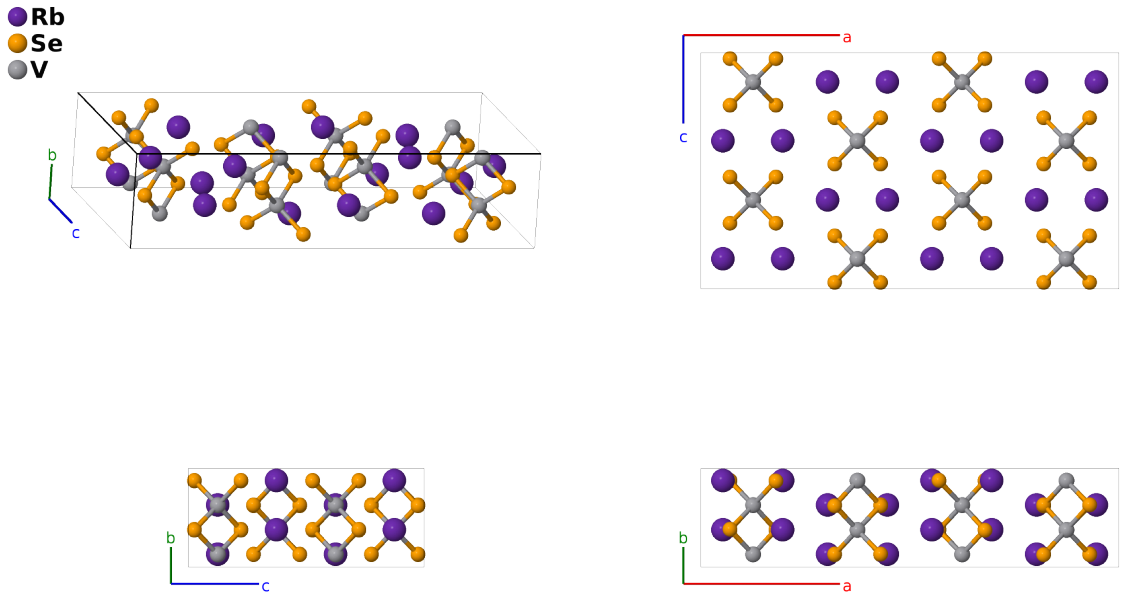
https://aflow.org/p/1RMB

https://aflow.org/p/AB2C_oF64_70_e_h_ab-001

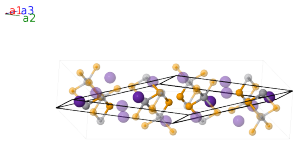


Prototype	$RbSe_2V$
AFLOW prototype label	AB2C_oF64_70_e_h_ab-001
ICSD	415479
Pearson symbol	oF64
Space group number	70
Space group symbol	$Fddd$
AFLOW prototype command	`aflow --proto=AB2C_oF64_70_e_h_ab-001 --params=`$a, b/a, c/a, x_3, x_4, y_4, z_4$

- Data for this structure was taken at 153K.
- We wish to thank Petra Lipsky, FIZ Karlsruhe - Leibniz-Institut für Informationsinfrastruktur, who provided us with the data referenced in (Deng, 2005). For more information about the FIZ Karlsruhe archive, see FIZ Karlsruhe.

Face-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(8a)	V I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}b\,\hat{\mathbf{y}} + \frac{7}{8}c\,\hat{\mathbf{z}}$	(8a)	V I
$\mathbf{B_3}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}b\,\hat{\mathbf{y}} + \frac{5}{8}c\,\hat{\mathbf{z}}$	(8b)	V II
$\mathbf{B_4}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(8b)	V II
$\mathbf{B_5}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Rb I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}b\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16e)	Rb I
$\mathbf{B_7}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Rb I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}b\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16e)	Rb I
$\mathbf{B_9}$	=	$\left(-x_4 + y_4 + z_4\right)\,\mathbf{a}_1 + \left(x_4 - y_4 + z_4\right)\,\mathbf{a}_2 + \left(x_4 + y_4 - z_4\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{10}}$	=	$\left(x_4 - y_4 + z_4\right)\,\mathbf{a}_1 + \left(-x_4 + y_4 + z_4\right)\,\mathbf{a}_2 - \left(x_4 + y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{11}}$	=	$\left(x_4 + y_4 - z_4\right)\,\mathbf{a}_1 - \left(x_4 + y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_4 + y_4 + z_4\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{12}}$	=	$-\left(x_4 + y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + y_4 - z_4\right)\,\mathbf{a}_2 + \left(x_4 - y_4 + z_4\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{13}}$	=	$\left(x_4 - y_4 - z_4\right)\,\mathbf{a}_1 - \left(x_4 - y_4 + z_4\right)\,\mathbf{a}_2 - \left(x_4 + y_4 - z_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{14}}$	=	$-\left(x_4 - y_4 + z_4\right)\,\mathbf{a}_1 + \left(x_4 - y_4 - z_4\right)\,\mathbf{a}_2 + \left(x_4 + y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{15}}$	=	$-\left(x_4 + y_4 - z_4\right)\,\mathbf{a}_1 + \left(x_4 + y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4 - y_4 - z_4\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B_{16}}$	=	$\left(x_4 + y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 + y_4 - z_4\right)\,\mathbf{a}_2 - \left(x_4 - y_4 + z_4\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32h)	Se I

References

[1] B. Deng, F. Q. Huang, D. E. Ellis, and J. A. Ibers, *Synthesis, crystal structure, and electronic structure of $RbVSe_2$*, J. Solid State Chem. **178**, 3251–3255 (2005), doi:10.1016/j.jssc.2005.08.004.