

RbVSe₂ Structure:

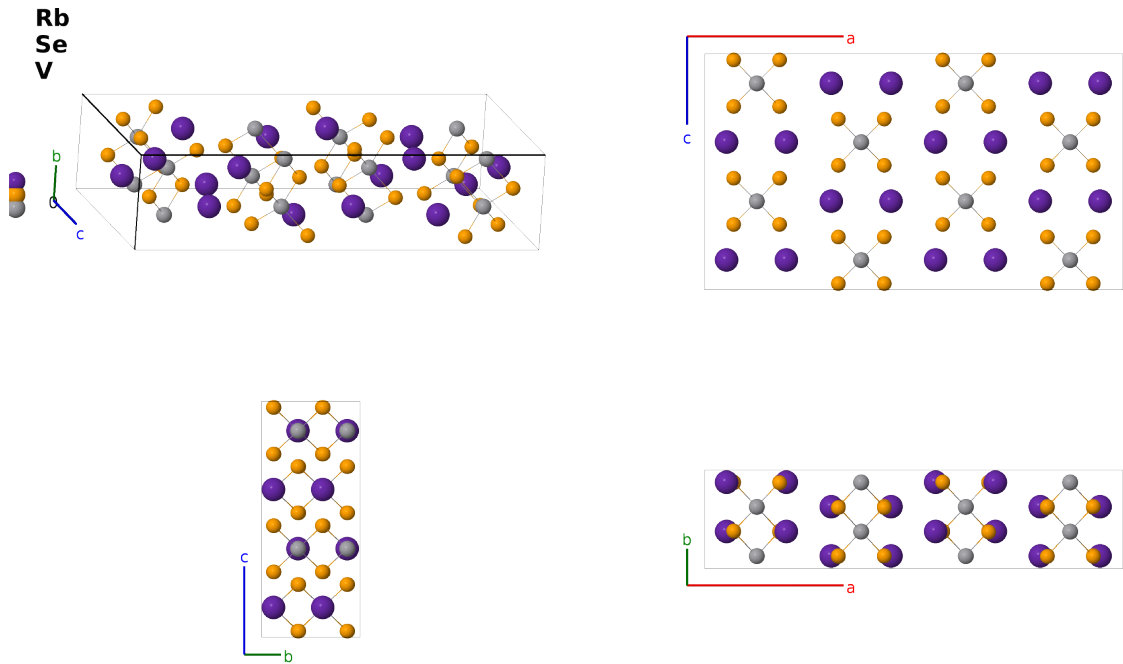
AB2C_oF64_70_e_h_ab-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/1RMB>

https://aflow.org/prototype-encyclopedia/AB2C_oF64_70_e_h_ab-001



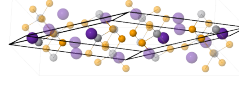
Prototype	RbSe ₂ V
AFLOW prototype label	AB2C_oF64_70_e_h_ab-001
ICSD	415479
CCDC	1729490
Pearson symbol	oF64
Space group number	70
Space group symbol	<i>Fddd</i>
AFLOW prototype command	<code>aflow --proto=AB2C_oF64_70_e_h_ab-001 --params=a, b/a, c/a, x₃, x₄, y₄, z₄</code>

- 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}\end{aligned}$$

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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
$\mathbf{B}_9$	$= (-x_4 + y_4 + z_4)\mathbf{a}_1 + (x_4 - y_4 + z_4)\mathbf{a}_2 + (x_4 + y_4 - z_4)\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} + by_4\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{10}$	$= (x_4 - y_4 + z_4)\mathbf{a}_1 + (-x_4 + y_4 + z_4)\mathbf{a}_2 - (x_4 + y_4 + z_4 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{4}\right)\hat{\mathbf{y}} + cz_4\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{11}$	$= (x_4 + y_4 - z_4)\mathbf{a}_1 - (x_4 + y_4 + z_4 - \frac{1}{2})\mathbf{a}_2 + (-x_4 + y_4 + z_4)\mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{4}\right)\hat{\mathbf{x}} + by_4\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{12}$	$= -(x_4 + y_4 + z_4 - \frac{1}{2})\mathbf{a}_1 + (x_4 + y_4 - z_4)\mathbf{a}_2 + (x_4 - y_4 + z_4)\mathbf{a}_3$	$=$	$ax_4\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{13}$	$= (x_4 - y_4 - z_4)\mathbf{a}_1 - (x_4 - y_4 + z_4)\mathbf{a}_2 - (x_4 + y_4 - z_4)\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} - by_4\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{14}$	$= -(x_4 - y_4 + z_4)\mathbf{a}_1 + (x_4 - y_4 - z_4)\mathbf{a}_2 + (x_4 + y_4 + z_4 + \frac{1}{2})\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{4}\right)\hat{\mathbf{y}} - cz_4\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{15}$	$= -(x_4 + y_4 - z_4)\mathbf{a}_1 + (x_4 + y_4 + z_4 + \frac{1}{2})\mathbf{a}_2 + (x_4 - y_4 - z_4)\mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{4}\right)\hat{\mathbf{x}} - by_4\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(32h)	Se I
$\mathbf{B}_{16}$	$= (x_4 + y_4 + z_4 + \frac{1}{2})\mathbf{a}_1 - (x_4 + y_4 - z_4)\mathbf{a}_2 - (x_4 - y_4 + z_4)\mathbf{a}_3$	$=$	$-ax_4\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(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.

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