

SrAl₂Se₄ Structure:

A2B4C_oC28_66_1_kl_a-001

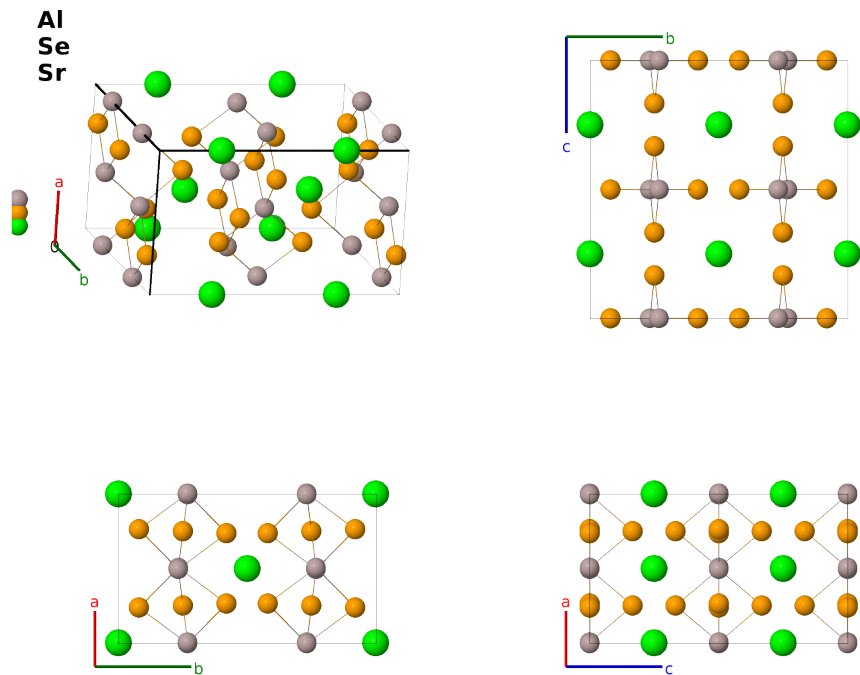
This structure previously used the label(s) **A2B4C_oC28_66_1_kl_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/QSR1>

https://aflow.org/prototype-encyclopedia/A2B4C_oC28_66_1_kl_a-001



Prototype	Al ₂ Se ₄ Sr
AFLOW prototype label	A2B4C_oC28_66_1_kl_a-001
ICSD	49732
CCDC	1614874
Pearson symbol	oC28
Space group number	66
Space group symbol	<i>Cccm</i>
AFLOW prototype command	<code>aflow --proto=A2B4C_oC28_66_1_kl_a-001</code> <code>--params=a, b/a, c/a, z₂, x₃, y₃, x₄, y₄</code>

Other compounds with this structure

CaAl₂Se₄

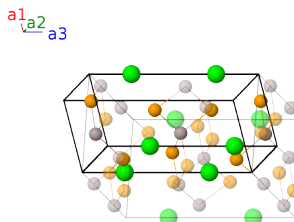
- We have shifted the origin so that the Sr-I atom is at the (4a) Wyckoff position rather than (4b).

Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}c \hat{\mathbf{z}}$	(4a)	Sr I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}c \hat{\mathbf{z}}$	(4a)	Sr I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8k)	Se I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	Se I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8k)	Se I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8k)	Se I
$\mathbf{B}_7$	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(8l)	Al I
$\mathbf{B}_8$	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(8l)	Al I
$\mathbf{B}_9$	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Al I
$\mathbf{B}_{10}$	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Al I
$\mathbf{B}_{11}$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(8l)	Se II
$\mathbf{B}_{12}$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(8l)	Se II
$\mathbf{B}_{13}$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Se II
$\mathbf{B}_{14}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8l)	Se II

References

- [1] W. Klee and H. Schäfer, *CaAl₂Se₄ und SrAl₂Se₄ — Strukturvarianten des TlSe-Typs*, Z. Naturforsch. B **33**, 829–833 (1978), doi:10.1515/znb-1978-0803.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043