# $SrSn_3$ Structure: A3B_hR16_166_2h_2c-001

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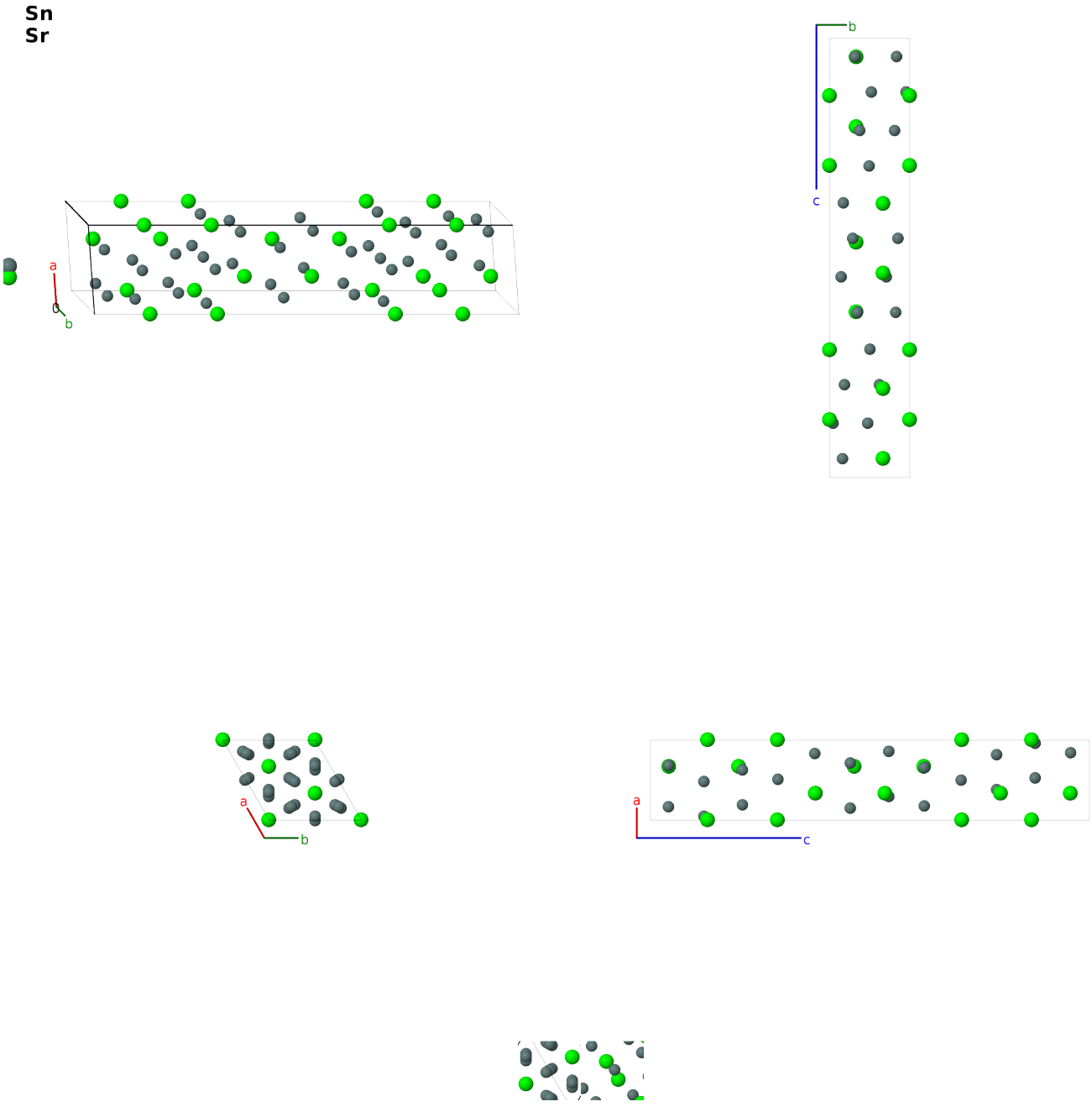
https://aflow.org/prototype-encyclopedia/X564

https://aflow.org/prototype-encyclopedia/A3B_hR16_166_2h_2c-001



| | |
|---|---|
| **Prototype** | $Sn_3Sr$ |
| **AFLOW prototype label** | A3B_hR16_166_2h_2c-001 |
| **ICSD** | 410956 |
| **CCDC** | 1726692 |
| **Pearson symbol** | hR16 |
| **Space group number** | 166 |
| **Space group symbol** | $R\bar{3}m$ |
| **AFLOW prototype command** | `aflow --proto=A3B_hR16_166_2h_2c-001 --params=`$a, c/a, x_1, x_2, x_3, z_3, x_4, z_4$ |

**Other compounds with this structure**
$BaPb_3$, $Ba(Sn, Bi)_3$, $DyGa_3$, $PuGa_3$

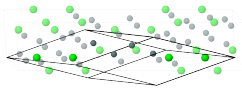
- The equilibrium phase diagram for the Sn-Sr system has been mapped by (Palenzona, 384):

| Formula | Structure |
|---|---|
| Sr | fcc ($A1$) |
| $Sr_2Sn$ | Cotunnite, $PbCl_2$ ($C23$) |
| $Sr_5Sn_3$ | $Cr_5B_3$ ($D8_l$) |
| SrSn | CrB ($B33$) |
| $Sr_3Sn_5$ | $Pd_5Pu_3$ |
| $SrSn_3$ | $SrSn_3$ (this structure) |
| $SrSn_4$ | $SrSn_4$ |
| Sn | diamond ($A4$) or $\beta$-Sn ($A5$) |

- $BaPb_3$ has also been found with small amounts calcium and strontium impurities on the barium sites.

**Rhombohedral primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$ | = | $cx_1\,\hat{\mathbf{z}}$ | (2c) | Sr I |
| $\mathbf{B_2}$ | = | $-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$ | = | $-cx_1\,\hat{\mathbf{z}}$ | (2c) | Sr I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$ | = | $cx_2\,\hat{\mathbf{z}}$ | (2c) | Sr II |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$ | = | $-cx_2\,\hat{\mathbf{z}}$ | (2c) | Sr II |

$$\mathbf{B_5} = x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_6} = z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_7} = x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3 = -\tfrac{1}{\sqrt{3}}a\,(x_3 - z_3)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_8} = -z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_3 - z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_9} = -x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 - z_3)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_3 - z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_{10}} = -x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3 = \tfrac{1}{\sqrt{3}}a\,(x_3 - z_3)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_3 + z_3)\;\hat{\mathbf{z}}$$ (6h) Sn I

$$\mathbf{B_{11}} = x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

$$\mathbf{B_{12}} = z_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

$$\mathbf{B_{13}} = x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3 = -\tfrac{1}{\sqrt{3}}a\,(x_4 - z_4)\;\hat{\mathbf{y}} + \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

$$\mathbf{B_{14}} = -z_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

$$\mathbf{B_{15}} = -x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_4 - z_4)\;\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

$$\mathbf{B_{16}} = -x_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3 = \tfrac{1}{\sqrt{3}}a\,(x_4 - z_4)\;\hat{\mathbf{y}} - \tfrac{1}{3}c\,(2x_4 + z_4)\;\hat{\mathbf{z}}$$ (6h) Sn II

## References


[1] T. F. Fässler and S. Hoffmann, *$SrSn_3$ - eine supraleitende Legierung mit freien Elektronenpaaren*, Z. Anorganische und Allgemeine Chemie **626**, 106–112 (2000), doi:10.1002/(SICI)1521-3749(200001)626:1<106::AID-ZAAC106>3.0.CO;2-W.

[2] A. Palenzona and M. Pani, *The phase diagram of the Sr-Sn system*, J. Alloys Compd. **384**, 227–230 (2004), doi:10.1016/j.jallcom.2004.04.097.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[1] S. Hoffmann and T. F. Fässler, *$SrSn_4$: A Superconducting Stannide with Localized and Delocalized Bond Character*, Inorg. Chem. **42**, 8748–8754 (2003), doi:10.1021/ic0302128.


## First cited in


N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).