# $FeSb_2$ Structure: AB2_oP6_34_a_c-001

This structure originally had the label `AB2_oP6_34_a_c`. Calls to that address will be redirected here.

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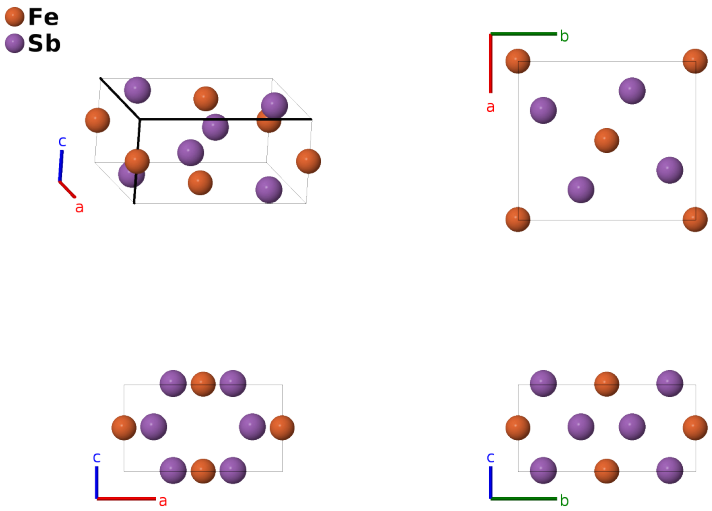
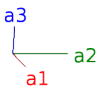
https://aflow.org/p/5KTQ

https://aflow.org/p/AB2_oP6_34_a_c-001

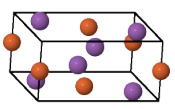



| | |
|---|---|
| **Prototype** | $FeSb_2$ |
| **AFLOW prototype label** | AB2_oP6_34_a_c-001 |
| **ICSD** | 15003 |
| **Pearson symbol** | oP6 |
| **Space group number** | 34 |
| **Space group symbol** | $Pnn2$ |
| **AFLOW prototype command** | `aflow --proto=AB2_oP6_34_a_c-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2$ |

**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 |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_3$ | = | $cz_1\,\hat{\mathbf{z}}$ | (2a) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (2a) | Fe I |
| $\mathbf{B_3}$ | = | $x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4c) | Sb I |
| $\mathbf{B_4}$ | = | $-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4c) | Sb I |
| $\mathbf{B_5}$ | = | $\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4c) | Sb I |
| $\mathbf{B_6}$ | = | $-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (4c) | Sb I |

**References**


[1] H. Holseth and A. Kjekshus, *Compounds with the Marcasite Type Crystal Structure. IV. The Crystal Structure of $FeSb_2$*, Acta Chem. Scand. **23**, 3043–3050 (1969), doi:10.3891/acta.chem.scand.23-3043.


**Found in**


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