# La $Se_{1.85}$ Structure: AB2_tP6_129_c_ac-003

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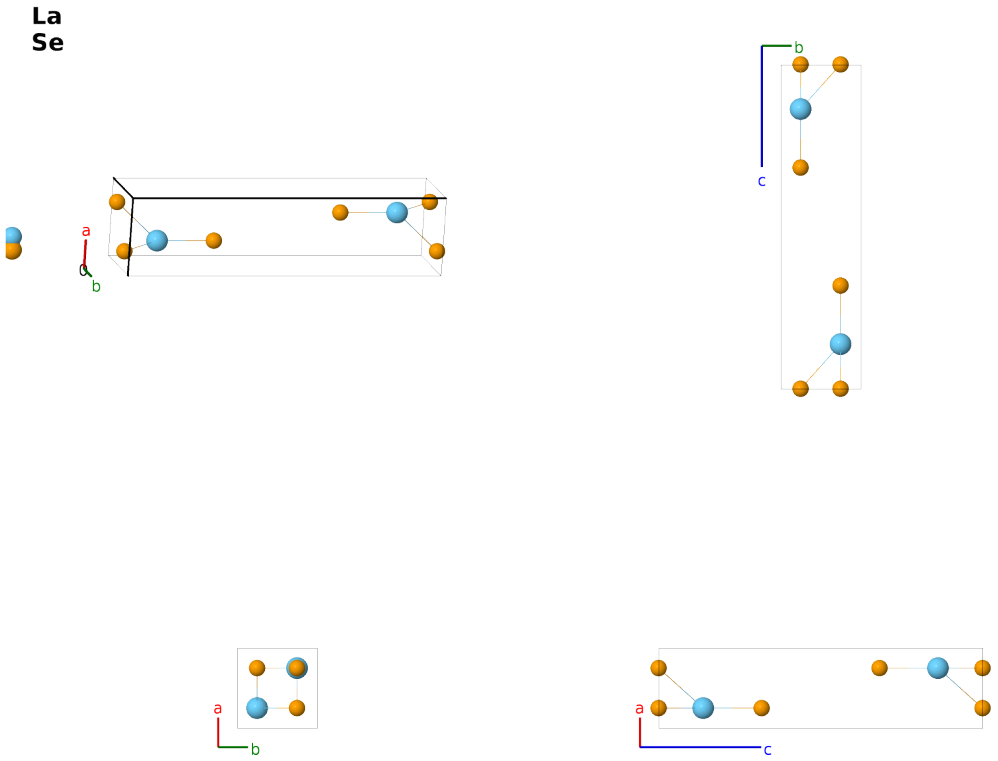
https://aflow.org/prototype-encyclopedia/2YWB

https://aflow.org/prototype-encyclopedia/AB2_tP6_129_c_ac-003




| | |
|---|---|
| **Prototype** | $LaSe_2$ |
| **AFLOW prototype label** | AB2_tP6_129_c_ac-003 |
| **ICSD** | 420787 |
| **CCDC** | 1733024 |
| **Pearson symbol** | tP6 |
| **Space group number** | 129 |
| **Space group symbol** | $P4/nmm$ |

**AFLOW prototype command** `aflow --proto=AB2_tP6_129_c_ac-003 --params=`$a, c/a, z_2, z_3$

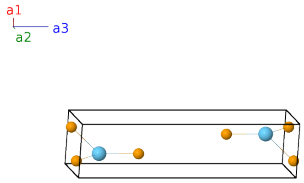
**Other compounds with this structure**

$CeSe_{1.83}$, $NdSe_{1.83}$, $SmSe_{1.84}$

- (Graf, 2009) find the selenium (2a) site to be occupied only 85.1% of the time, giving the observed stoichiometry. They took the data for this structure at 130K.
- $Cu_2Sb$ ($C38$), $UP_2$, and $LaSe_{1.85}$ have similar AFLOW prototype labels, A2B_tP6_129_ac_c for the first two and AB2_tP6_129_c_ac for the third. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We consider all of these to be binary forms of Matlockite ($E0_1$)/PrOI.
- We somewhat arbitrarily assign
  - Structures with c/a $< 2$ to the $Cu_2Sb$ prototype,
  - Structures with $2 <$ c/a $< 3$ to the $UP_2$ prototype, and
  - Structures with c/a $\approx 4$ to the $LaSe_{1.85}$ prototype.

**Simple Tetragonal primitive vectors**

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$ | (2a) | Se I |
| $\mathbf{B_2}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$ | (2a) | Se I |
| $\mathbf{B_3}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2c) | La I |
| $\mathbf{B_4}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2c) | La I |
| $\mathbf{B_5}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2c) | Se II |
| $\mathbf{B_6}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2c) | Se II |

**References**


[1] C. Graf and T. Doert, *$LaSe_{1.85}$, $CeSe_{1.83}$, $NdSe_{1.83}$ and $SmSe_{1.84}$ - Four new polychalcogenides of the rare earth metals with incommensurate site occupancy and displacive modulation* **224**, 568–579 (2009), doi:10.1524/zkri.2009.1197.

**Found in**

[1] *Inorganic Crystal Structure Database*. Entry 420787 ($LaSe_{1.85}$).

**First cited in**

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