# $RbAlF_4$ III Structure: AB4C_oP24_59_c_efg_ab-001

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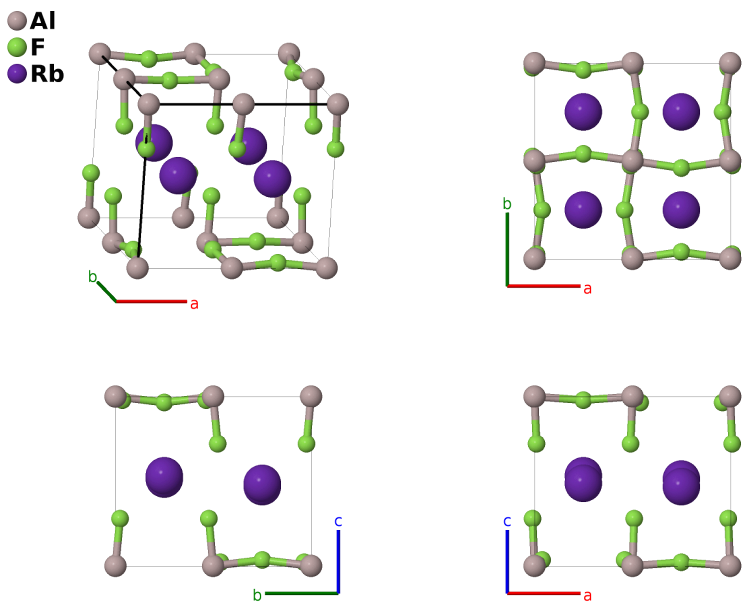
https://aflow.org/p/Q57Q

https://aflow.org/p/AB4C_oP24_59_c_efg_ab-001




| | |
|---|---|
| **Prototype** | $AlF_4Rb$ |
| **AFLOW prototype label** | AB4C_oP24_59_c_efg_ab-001 |
| **ICSD** | 54123 |
| **Pearson symbol** | oP24 |
| **Space group number** | 59 |
| **Space group symbol** | $Pmmn$ |
| **AFLOW prototype command** | `aflow --proto=AB4C_oP24_59_c_efg_ab-001` `--params=`$a, b/a, c/a, z_1, z_2, y_4, z_4, x_5, z_5, x_6, y_6, z_6$ |

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**Other compounds with this structure**

$CsVF_4$ IV, $RbFeF_4$ II

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- (Bulou, 1982) identify three phases of $RbAlF_4$:
  - Above 553K $RbAlF_4$ I has the tetragonal $TlAlF_4$ ($H0_8$) structure.
  - Between 282 and 553K $RbAlF_4$ II is tetragonal, space group $P4/mbm$ #127.
  - Below 282K $RbAlF_4$ III is orthorhombic, space group $Pmmn$ #59 (this structure).
- The different structures are distinguished by the tilt of the $AlF_6$ octahedra.

- We use Bulou and Nouet's data for $RbAlF_4$ III at 5K.

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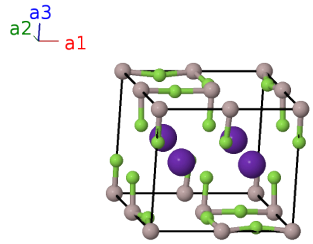
### Simple Orthorhombic primitive vectors

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

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### Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (2a) | Rb I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$ | (2a) | Rb I |
| $\mathbf{B_3}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2b) | Rb II |
| $\mathbf{B_4}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2b) | Rb II |
| $\mathbf{B_5}$ | = | $0$ | = | $0$ | (4c) | Al I |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$ | (4c) | Al I |
| $\mathbf{B_7}$ | = | $\frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}b\,\hat{\mathbf{y}}$ | (4c) | Al I |
| $\mathbf{B_8}$ | = | $\frac{1}{2}\,\mathbf{a}_1$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}}$ | (4c) | Al I |
| $\mathbf{B_9}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4e) | F I |
| $\mathbf{B_{10}}$ | = | $\frac{1}{4}\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4e) | F I |
| $\mathbf{B_{11}}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4e) | F I |
| $\mathbf{B_{12}}$ | = | $\frac{3}{4}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4e) | F I |
| $\mathbf{B_{13}}$ | = | $x_5\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4f) | F II |
| $\mathbf{B_{14}}$ | = | $-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4f) | F II |
| $\mathbf{B_{15}}$ | = | $-x_5\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (4f) | F II |
| $\mathbf{B_{16}}$ | = | $\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (4f) | F II |
| $\mathbf{B_{17}}$ | = | $x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{18}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{19}}$ | = | $-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{20}}$ | = | $\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{21}}$ | = | $-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{22}}$ | = | $\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{23}}$ | = | $x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |
| $\mathbf{B_{24}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | F III |

## References


[1] A. Bulou and J. Nouet, *Structural phase transitions in ferroelastic $RbAlF_4$. I. DSC, X-ray powder diffraction investigations and neutron powder profile refinement of the structures*, J. Phys. C: Solid State Phys. **15**, 183–196 (1982), doi:10.1088/0022-3719/15/2/004.