

RbAlF₄ III Structure:

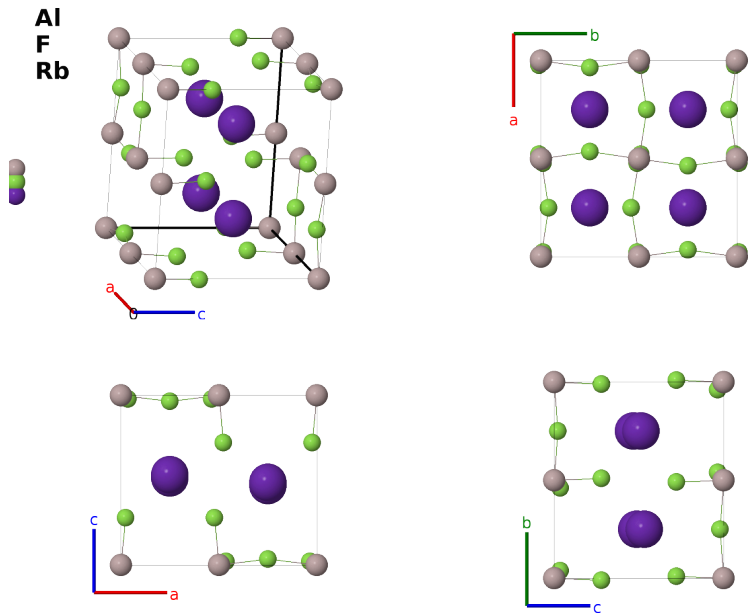
AB4C_oP24_59_c_efg_ab-001

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<https://aflow.org/prototype-encyclopedia/Q57Q>

https://aflow.org/prototype-encyclopedia/AB4C_oP24_59_c_efg_ab-001



Prototype	AlF ₄ Rb
AFLOW prototype label	AB4C_oP24_59_c_efg_ab-001
ICSD	54123
CCDC	1618725
Pearson symbol	oP24
Space group number	59
Space group symbol	<i>Pm</i> <i>mn</i>
AFLOW prototype command	<code>aflow --proto=AB4C_oP24_59_c_efg_ab-001</code> <code>--params=a, b/a, c/a, z₁, z₂, y₄, z₄, x₅, z₅, x₆, y₆, z₆</code>

Other compounds with this structure

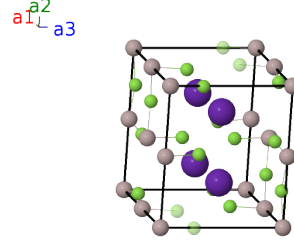
CsVF₄ IV, RbFeF₄ II

- (Bulou, 1982) identify three phases of RbAlF₄:
 - Above 553K RbAlF₄ I has the tetragonal TlAlF₄ (*H*0₈) 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.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_{10}$	$= \frac{1}{4} \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B}_{11}$	$= \frac{3}{4} \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{16}$	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{19}$	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{20}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8g)	F III
$\mathbf{B}_{23}$	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8g)	F III

$$\mathbf{B}_{24} = -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 = -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} \quad (8g) \quad \text{F III}$$

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.

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