

RbAlF₄ II Structure:

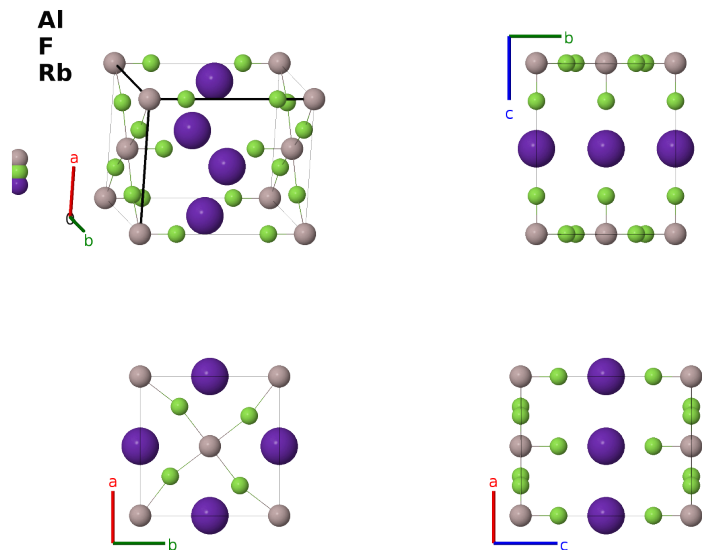
AB4C_tP12_127_a_eg_c-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/QJN8>

https://aflow.org/prototype-encyclopedia/AB4C_tP12_127_a_eg_c-001



Prototype	AlF ₄ Rb
AFLOW prototype label	AB4C_tP12_127_a_eg_c-001
ICSD	54121
CCDC	1618723
Pearson symbol	tP12
Space group number	127
Space group symbol	<i>P4/mbm</i>
AFLOW prototype command	<code>aflow --proto=AB4C_tP12_127_a_eg_c-001 --params=a, c/a, z₃, x₄</code>

- (Bulou, 1982) identify three phases of RbAlF₄:
 - Above 553K RbAlF₄ I has the tetragonal TlAlF₄ (*H0₈*) structure.
 - Between 282 and 553K RbAlF₄ II is tetragonal, space group *P4/mbm* #127 (this structure).
 - Below 282K RbAlF₄ III is orthorhombic, space group *Pmmn* #59.
- The different structures are distinguished by the tilt of the AlF₆ octahedra.

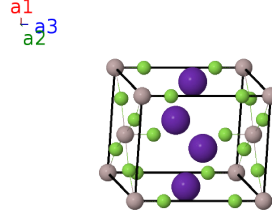
- We use Bulou and Nouet's data for RbAlF_4 II at 293K.

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
$\mathbf{B}_1$	$=$	0	$=$	0	Al I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	Al I
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	Rb I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	Rb I
$\mathbf{B}_5$	$=$	$z_3 \mathbf{a}_3$	$=$	$c z_3 \hat{\mathbf{z}}$	F I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	F I
$\mathbf{B}_7$	$=$	$-z_3 \mathbf{a}_3$	$=$	$-c z_3 \hat{\mathbf{z}}$	F I
$\mathbf{B}_8$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	F I
$\mathbf{B}_9$	$=$	$x_4 \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$a x_4 \hat{\mathbf{x}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{y}}$	F II
$\mathbf{B}_{10}$	$=$	$-x_4 \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$-a x_4 \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}}$	F II
$\mathbf{B}_{11}$	$=$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}}$	F II
$\mathbf{B}_{12}$	$=$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$a (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}}$	F II

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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