$RbAlF_4$ II Structure: AB4C_tP12_127_a_eg_c-001

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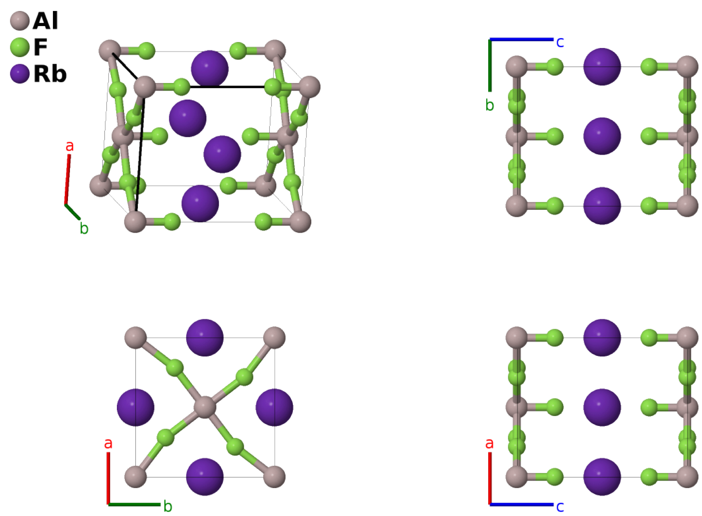
https://aflow.org/p/QJN8

https://aflow.org/p/AB4C_tP12_127_a_eg_c-001

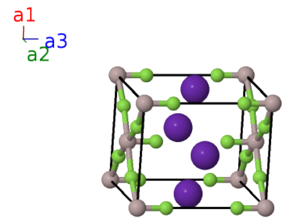


Prototype	AlF_4Rb
AFLOW prototype label	AB4C_tP12_127_a_eg_c-001
ICSD	54121
Pearson symbol	tP12
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=AB4C_tP12_127_a_eg_c-001` `--params=`$a, c/a, z_3, x_4$

- (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 (this structure).
  - Below 282K $RbAlF_4$ III is orthorhombic, space group $Pmmn$ #59.
- The different structures are distinguished by the tilt of the AlF_6 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	(2a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(2a)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Rb I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Rb I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_{11}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(4g)	F II
$\mathbf{B_{12}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(4g)	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.