$RbPaF_6$ (V) Structure: A6BC_oC32_67_no_c_g-001

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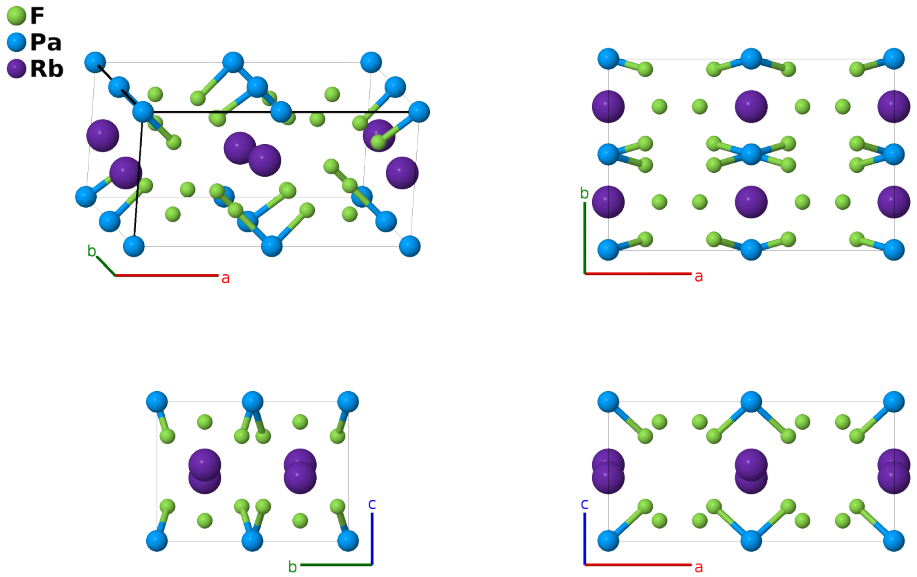
https://aflow.org/p/PLRV

https://aflow.org/p/A6BC_oC32_67_no_c_g-001



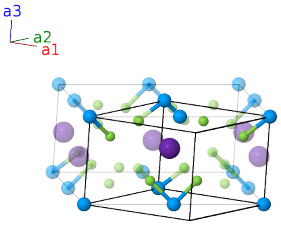
Prototype	$RbPaF_6$
AFLOW prototype label	A6BC_oC32_67_no_c_g-001
ICSD	36078
Pearson symbol	oC32
Space group number	67
Space group symbol	*Cmme*
AFLOW prototype command	`aflow --proto=A6BC_oC32_67_no_c_g-001 --params=`$a, b/a, c/a, z_2, x_3, z_3, x_4, y_4, z_4$

Other compounds with this structure
$SrTbF_6$

- (Burns, 1968) assign the protactinium atom to the (4b) Wyckoff site, but give coordinates for the (4e) site. We use these coordinates and assign the Wyckoff position appropriately. The axis orientation has been adjusted by AFLOW.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4c)	Pa I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Pa I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4g)	Rb I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4g)	Rb I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8n)	F I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8n)	F I
$\mathbf{B_7}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8n)	F I
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8n)	F I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{10}}$	=	$\left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{11}}$	=	$-\left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{13}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{14}}$	=	$\left(x_4 - y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{15}}$	=	$\left(x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 - y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16o)	F II
$\mathbf{B_{16}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16o)	F II

References

[1] J. H. Burns, H. A. Levy, and J. O. L. Keller, *The crystal structure of rubidium hexafluoroprotactinate(V), $RbPaF_6$*, Acta Crystallogr. Sect. B **24**, 1675–1680 (1968), doi:10.1107/S0567740868004838.