KPF_6 Structure: A24BC_cF104_209_j_a_b-001

This structure previously used the label(s) `A24BC_cF104_209_j_a_b`. Calls to these addresses will be redirected here.

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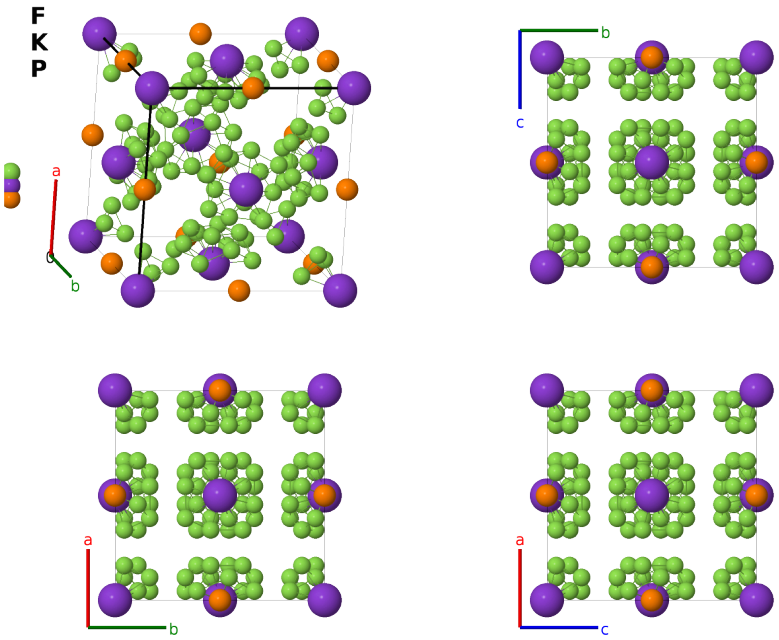
https://aflow.org/prototype-encyclopedia/XBGM

https://aflow.org/prototype-encyclopedia/A24BC_cF104_209_j_a_b-001

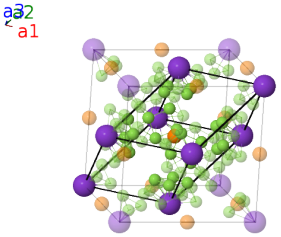


Prototype	F_6KP
AFLOW prototype label	A24BC_cF104_209_j_a_b-001
Pearson symbol	cF104
Space group number	209
Space group symbol	$F432$
AFLOW prototype command	`aflow --proto=A24BC_cF104_209_j_a_b-001 --params=`a, x_3, y_3, z_3

- The (96j) Wyckoff positions are decorated by F atoms with a site occupation of 0.25, hence the prototype material is KPF_6 rather than KPF_{24}.

Face-centered Cubic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_3}$	=	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 - y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_4}$	=	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 - (x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_5}$	=	$(x_3 + y_3 - z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_6}$	=	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_7}$	=	$(x_3 + y_3 - z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_8}$	=	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 - y_3 + z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_9}$	=	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 - (x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{10}}$	=	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{11}}$	=	$(x_3 - y_3 + z_3)\,\mathbf{a}_1 + (x_3 + y_3 - z_3)\,\mathbf{a}_2 + (-x_3 + y_3 + z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{12}}$	=	$(-x_3 + y_3 + z_3)\,\mathbf{a}_1 - (x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 - y_3 + z_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{13}}$	=	$-(x_3 + y_3 + z_3)\,\mathbf{a}_1 + (-x_3 + y_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3 - z_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96j)	F I

$\mathbf{B_{14}}$	=	$(x_3 + y_3 - z_3)\ \mathbf{a}_1 +$ $(x_3 - y_3 + z_3)\ \mathbf{a}_2 -$ $(x_3 + y_3 + z_3)\ \mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{15}}$	=	$(x_3 - y_3 - z_3)\ \mathbf{a}_1 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_2 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{16}}$	=	$-(x_3 - y_3 + z_3)\ \mathbf{a}_1 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_2 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{17}}$	=	$-(x_3 + y_3 - z_3)\ \mathbf{a}_1 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_2 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{18}}$	=	$(x_3 + y_3 + z_3)\ \mathbf{a}_1 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_2 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{19}}$	=	$-(x_3 + y_3 - z_3)\ \mathbf{a}_1 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_2 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{20}}$	=	$(x_3 + y_3 + z_3)\ \mathbf{a}_1 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_2 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{21}}$	=	$(x_3 - y_3 - z_3)\ \mathbf{a}_1 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_2 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{22}}$	=	$-(x_3 - y_3 + z_3)\ \mathbf{a}_1 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_2 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{23}}$	=	$-(x_3 - y_3 + z_3)\ \mathbf{a}_1 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_2 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{24}}$	=	$(x_3 - y_3 - z_3)\ \mathbf{a}_1 +$ $(x_3 + y_3 + z_3)\ \mathbf{a}_2 -$ $(x_3 + y_3 - z_3)\ \mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{25}}$	=	$(x_3 + y_3 + z_3)\ \mathbf{a}_1 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_2 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(96j)	F I
$\mathbf{B_{26}}$	=	$-(x_3 + y_3 - z_3)\ \mathbf{a}_1 -$ $(x_3 - y_3 + z_3)\ \mathbf{a}_2 +$ $(x_3 - y_3 - z_3)\ \mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(96j)	F I

References

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

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