$PrRu_4P_{12}$ Structure: A12BC4_cP34_195_2j_ab_2e-001

This structure originally had the label `A12BC4_cP34_195_2j_ab_2e`. Calls to that address will be redirected here.

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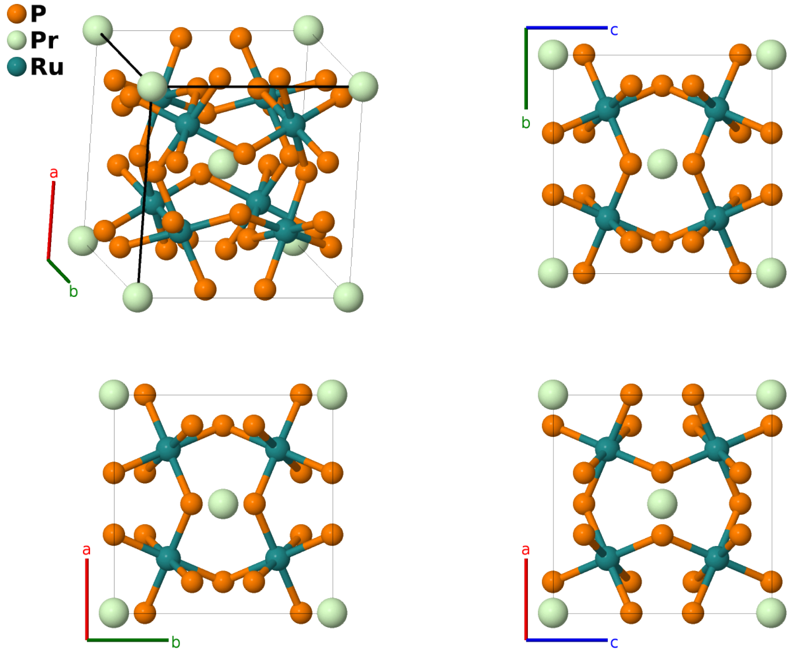
https://aflow.org/p/8SJC

https://aflow.org/p/A12BC4_cP34_195_2j_ab_2e-001



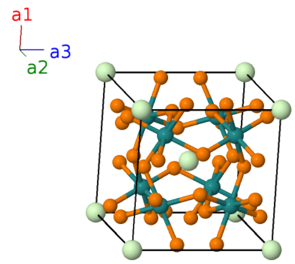
Prototype	$P_{12}PrRu_4$
AFLOW prototype label	A12BC4_cP34_195_2j_ab_2e-001
ICSD	55834
Pearson symbol	cP34
Space group number	195
Space group symbol	$P23$
AFLOW prototype command	`aflow --proto=A12BC4_cP34_195_2j_ab_2e-001` `--params=`$a, x_3, x_4, x_5, y_5, z_5, x_6, y_6, z_6$

- (Lee, 2004) give two refinements of this structure, in space group $P23$ #195 and space group $Pm\bar{3}$ #200, both with the same R factor. We show the results for $P23$. AFLOW the difference between the two structures to be quite small.
- Using its default tolerance, AFLOW places this structure in space group $Im\bar{3}$ #204, with all the atoms of a given species located on one Wyckoff position. It is likely that first-principles calculations will relax into that space group.
- The reported $P23$ structure can be recovered using the commmand

- aflow --proto=A12BC4_cP34_195_2j_ab_2e:P:Pr:Ru --params=a,x_3,x_4,x_5,y_5,z_5,x_6,y_6,z_6 --tolerance=0.001.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pr I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Pr II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4e)	Ru I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B_{10}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4e)	Ru II
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{13}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{14}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{15}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{16}}$	=	$z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{17}}$	=	$-z_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{18}}$	=	$-z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - y_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ay_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{19}}$	=	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{20}}$	=	$-y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{21}}$	=	$y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{22}}$	=	$-y_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(12j)	P I
$\mathbf{B_{23}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{24}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + az_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{25}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{26}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - az_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{27}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	P II

$\mathbf{B_{28}}$	=	$z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{29}}$	=	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + ay_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{30}}$	=	$-z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - y_6\,\mathbf{a}_3$	=	$-az_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - ay_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{31}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{32}}$	=	$-y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{33}}$	=	$y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} - ax_6\,\hat{\mathbf{z}}$	(12j)	P II
$\mathbf{B_{34}}$	=	$-y_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} - az_6\,\hat{\mathbf{y}} + ax_6\,\hat{\mathbf{z}}$	(12j)	P II

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