

PrRu₄P₁₂ Structure: A12BC4_cP34_195_2j_ab_2e-001

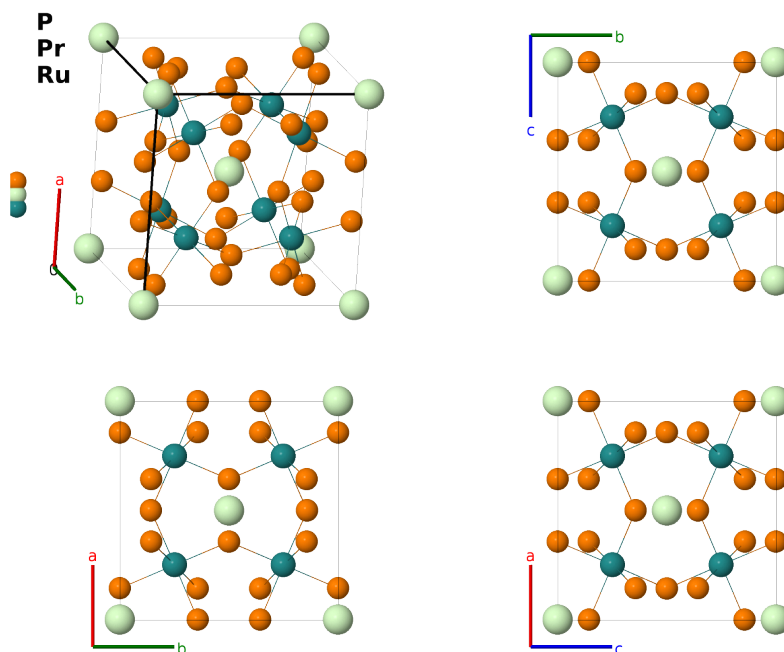
This structure previously used the label(s) **A12BC4_cP34_195_2j_ab_2e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/8SJC>

https://aflow.org/prototype-encyclopedia/A12BC4_cP34_195_2j_ab_2e-001



Prototype	P ₁₂ PrRu ₄
AFLOW prototype label	A12BC4_cP34_195_2j_ab_2e-001
ICSD	55834
CCDC	1620131
Pearson symbol	cP34
Space group number	195
Space group symbol	<i>P</i> 23
AFLOW prototype command	<code>aflow --proto=A12BC4_cP34_195_2j_ab_2e-001</code> <code>--params=a, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- (Lee, 2004) give two refinements of this structure, in space group *P*23 #195 and space group *Pm* $\bar{3}$ #200, both with the same *R* factor. We show the results for *P*23, as it is the lesser-known space group. The ICSD entry is for the higher symmetry space group.

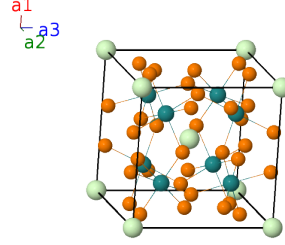
- The difference between the two structures to be quite small.
- Using its default tolerance, AFLOW places this structure in space group $Im\bar{3}$ #204, with all the atoms of a given species located on one Wyckoff position. It is likely that first-principles calculations will relax into that space group.
- The reported $P23$ structure can be recovered using the command
- `afLOW --proto=A12BC4.cP34_195_2j.ab_2e:P:Pr:Ru --params=a,x3,x4,x5,y5,z5,x6,y6,z6 --tolerance=0.001.`
- Space group $P23$ #195 is chiral, Sohncke Class III, so this structure could be found in a mirror image configuration in the same space group, but with the default tolerance both space groups would revert to the same $Im\bar{3}$ structure.

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

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{P II}
\end{aligned}$$

References

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