Rb_2P_3 Structure: A3B2_oF40_69_hm_fg-001

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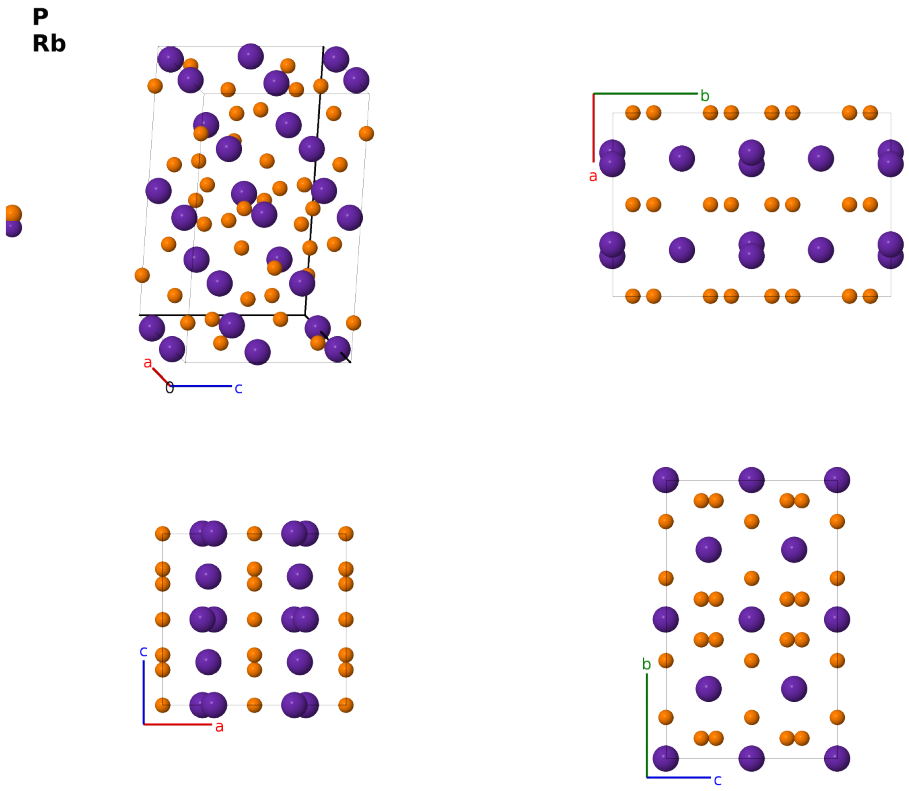
https://aflow.org/prototype-encyclopedia/QBNS

https://aflow.org/prototype-encyclopedia/A3B2_oF40_69_hm_fg-001



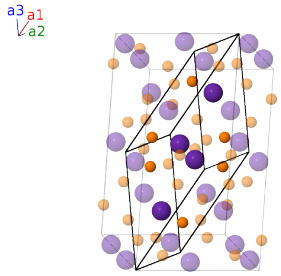
Prototype	P_3Rb_2
AFLOW prototype label	A3B2_oF40_69_hm_fg-001
ICSD	65184
CCDC	1160102
Pearson symbol	oF40
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=A3B2_oF40_69_hm_fg-001 --params=`$a, b/a, c/a, x_2, y_3, y_4, z_4$

Other compounds with this structure

Cs_2P_3

Face-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8f)	Rb I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8f)	Rb I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(8g)	Rb II
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(8g)	Rb II
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B_6}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}$	(8h)	P I
$\mathbf{B_7}$	=	$(y_4 + z_4)\,\mathbf{a}_1 - (y_4 - z_4)\,\mathbf{a}_2 + (y_4 - z_4)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16m)	P II
$\mathbf{B_8}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 - (y_4 + z_4)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16m)	P II
$\mathbf{B_9}$	=	$(y_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16m)	P II
$\mathbf{B_{10}}$	=	$-(y_4 + z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16m)	P II

References

[1] H. G. von Schnering, T. Meyer, W. Hönle, W. Bauhofer, G. Kliche, T. Meyer, W. Schmettow, U. Hinze, W. Bauhofer, and G. Kliche, *Zur Chemie und Strukturchemie von Phosphiden und Polyphosphiden. 46. Tetrarubidiumhexaphosphid und Tetracäsiumhexaphosphid: Darstellung, Struktur und Eigenschaften von Rb_4P_6 und Cs_4P_6*, Z. Anorganische und Allgemeine Chemie **553**, 261–279 (1987), doi:10.1002/zaac.19875531031.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*, vol. 4 (ASM International, Materials Park, OH, 1991), 2nd edn.

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