$K_2RbSc(PO_4)_2$ Structure: A2B8C2DE_hP14_164_d_di_d_a_b-001

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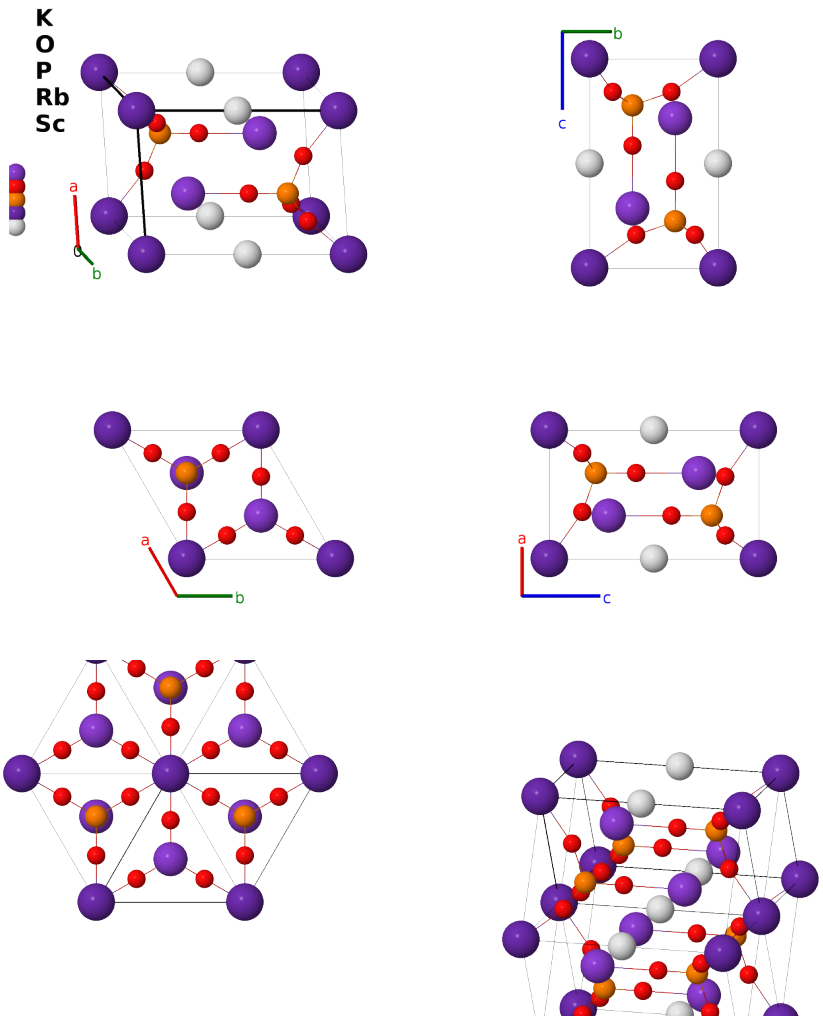
https://aflow.org/prototype-encyclopedia/8UWN

https://aflow.org/prototype-encyclopedia/A2B8C2DE_hP14_164_d_di_d_a_b-001



Prototype	$K_2O_8P_2RbSc$
AFLOW prototype label	A2B8C2DE_hP14_164_d_di_d_a_b-001
ICSD	148290
CCDC	2261864
Pearson symbol	hP14
Space group number	164

Space group symbol $P\bar{3}m1$

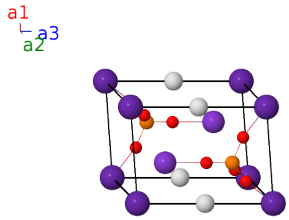
AFLOW prototype command `aflow --proto=A2B8C2DE_hP14_164_d_di_d_a_b-001 --params=`$a, c/a, z_3, z_4, z_5, x_6, z_6$

Other compounds with this structure
$K_2CsYb(PO_4)_2$, $Rb_3Er(PO_4)_2$, $Rb_3Lu(PO_4)_2$, $Rb_3Yb(PO_4)_2$

- The ICSD lists $KAl(MoO_4)_2$ as the structure type for these compounds, but the addition of an additional atomic species on a new (2d) site requires a new AFLOW prototype. We arbitrarily chose $K_2RbSc(PO_4)_2$ as the representative compound.
- $K_2RbSc(PO_4)_2$ and $Na_2BaMn(VO_4)_2$ occupy the same Wyckoff positions in space grop $P\bar{3}m1$ #164, but their AFLOW mismatch (Hicks, 2018) is sufficiently large (0.35) that we place them in two different prototypes. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Rb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Sc I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	K I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	K I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2d)	P I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2d)	P I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + 2x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B_{11}}$	=	$-2x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B_{13}}$	=	$2x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	O II
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 - 2x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6i)	O II

References

[1] J. Zhou, P. Gong, M. Xia, and Q. Wu, *Co-substitution design: a new glaserite-type rare-earth phosphate $K_2RbSc(PO_4)_2$ with high structural tolerance*, Dalton Trans. **52**, 15807–15814 (2023), doi:10.1039/D3DT02494F.

[2] D. Hicks, C. Oses, E. Gossett, G. Gomez, R. H. Taylor, C. Toher, M. J. Mehl, O. Levy, and S. Curtarolo, *AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals*, Acta Crystallogr. Sect. A **74**, 184–203 (2018), doi:10.1107/S2053273318003066.

Found in

[1] *Inorganic Crystal Structure Database*. Entry 148290 [K2RbSc(PoO4)2].

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