$KNaSO_4$ Structure: ABC4D_hP14_156_ac_bc_ab2d_ab-001

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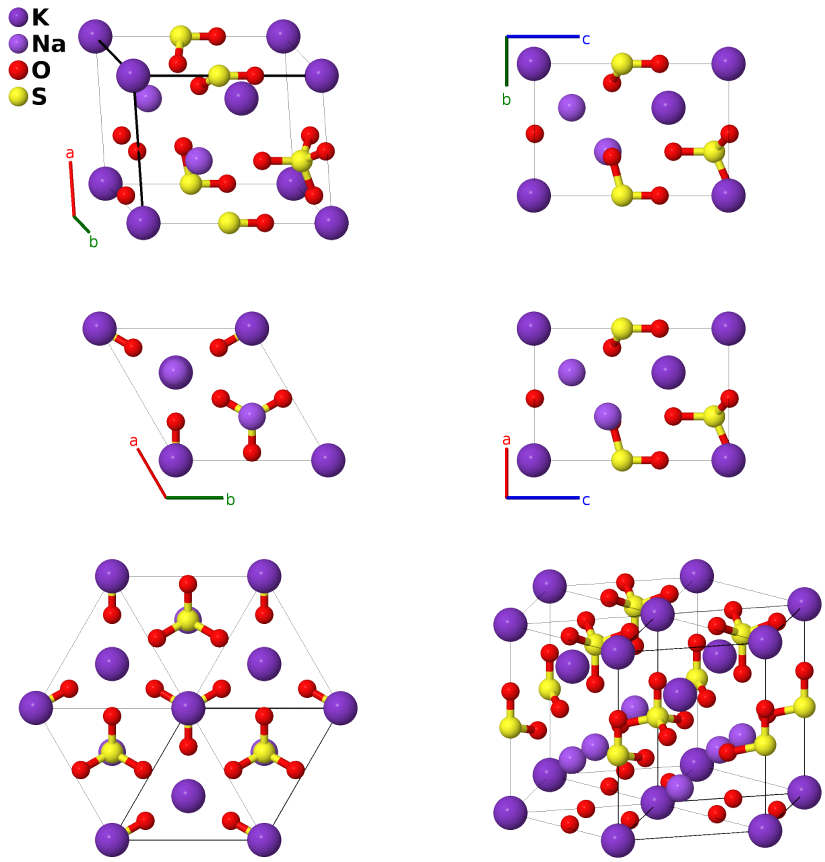
https://aflow.org/p/Z1Y1

https://aflow.org/p/ABC4D_hP14_156_ac_bc_ab2d_ab-001



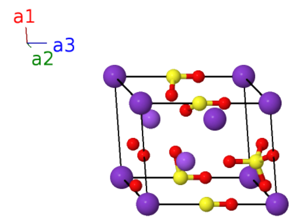
Prototype	$KNaO_4S$
AFLOW prototype label	ABC4D_hP14_156_ac_bc_ab2d_ab-001
ICSD	133733
Pearson symbol	hP14
Space group number	156
Space group symbol	$P3m1$
AFLOW prototype command	`aflow --proto=ABC4D_hP14_156_ac_bc_ab2d_ab-001` `--params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, x_9, z_9, x_{10}, z_{10}$

- We have shifted the origin so that the atom (Okada, 1980) label K(2) is at the origin. Note that space group $P3m1$ #156 allows an arbitrary origin for the z-axis. In addition, the origin can be shifted so that (1b) or (1c) atoms are moved to the origin.

- There is no ICSD for the (Okada, 1980) structure of $KNaSO_4$, although the ICSD has entries for $K_3Na(SO_4)_2$ from the same paper. We provide the ICSD entry from the later work of (Filatov, 2019), who named the mineral form belomarinaite.
- Belomarinaite has some mixture of sodium and potassium on the (1a) and (1c) sites that was not reported by (Okada, 1980).

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	K I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	O I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(1a)	S I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1b)	Na I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(1b)	O II
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(1b)	S II
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(1c)	K II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(1c)	Na II
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-\sqrt{3}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{10}}$	=	$x_9\,\mathbf{a}_1 + 2x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{3}{2}ax_9\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{11}}$	=	$-2x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_9\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(3d)	O III
$\mathbf{B_{12}}$	=	$x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B_{13}}$	=	$x_{10}\,\mathbf{a}_1 + 2x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV
$\mathbf{B_{14}}$	=	$-2x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(3d)	O IV

References

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