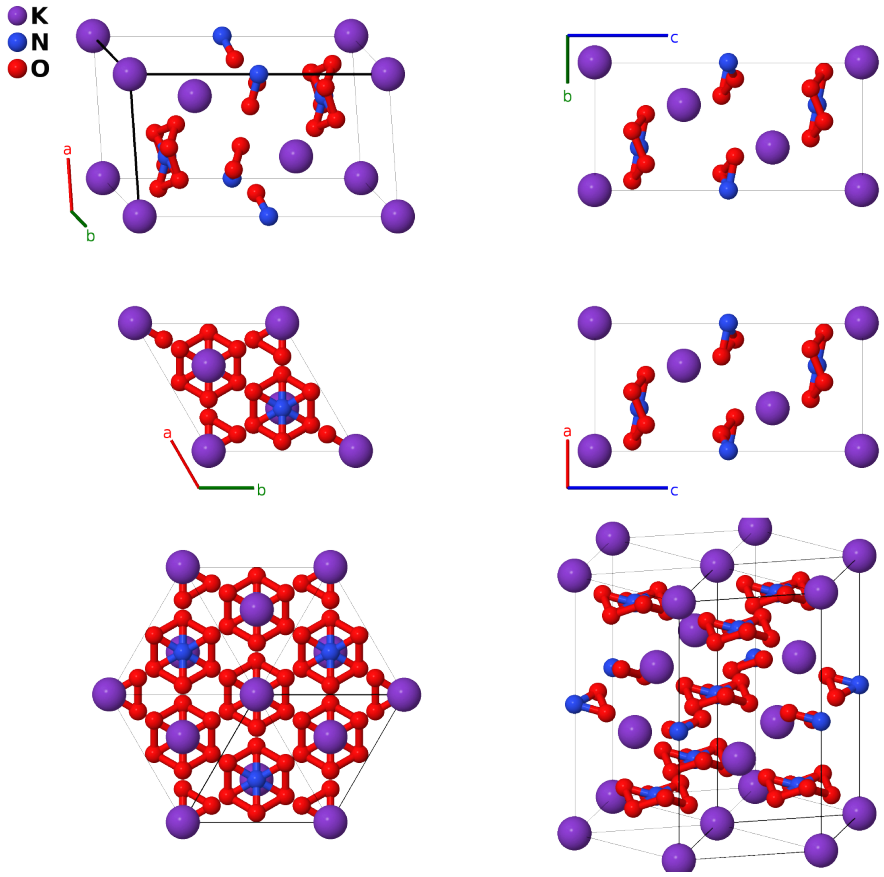
β-Potassium Nitrate (KNO_3) Structure: ABC6_hR8_166_a_b_h-001

This structure originally had the label `ABC6_hR8_166_a_b_h`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/XD6C

https://aflow.org/p/ABC6_hR8_166_a_b_h-001

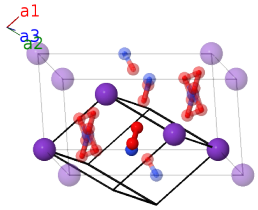


Prototype	KNO_3
AFLOW prototype label	ABC6_hR8_166_a_b_h-001
ICSD	385
Pearson symbol	hR8
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC6_hR8_166_a_b_h-001 --params=`$a, c/a, x_3, z_3$

- On heating, α-KNO_3 (either Structure I or Structure II) transforms into β-KNO_3 at 128°C. When heated above 200°C and then cooled, the β phase transforms into the metastable ferroelectric γ-KNO_3 phase, which can remain down to room temperature.
- In the β-phase the oxygen (6h) sites are only 50% filled. Presumably only the $+z$ or $-z$ sites will be occupied around a given nitrogen atom.
- We use the 151°C data from (Nimmo, 1976).

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	N I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(6h)	O I

References

[1] J. K. Nimmo and B. W. Lucas, *The crystal structures of γ-and β-KNO3 and the α-β-γ phase transformations*, Acta Crystallogr. Sect. B **32** (1976), doi:10.1107/S0567740876006894.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).