γ-Potassium Nitrate (KNO_3) Structure: ABC3_hR5_160_a_a_b-002

This structure originally had the label `ABC3_hR5_160_a_a_b`. Calls to that address will be redirected here.

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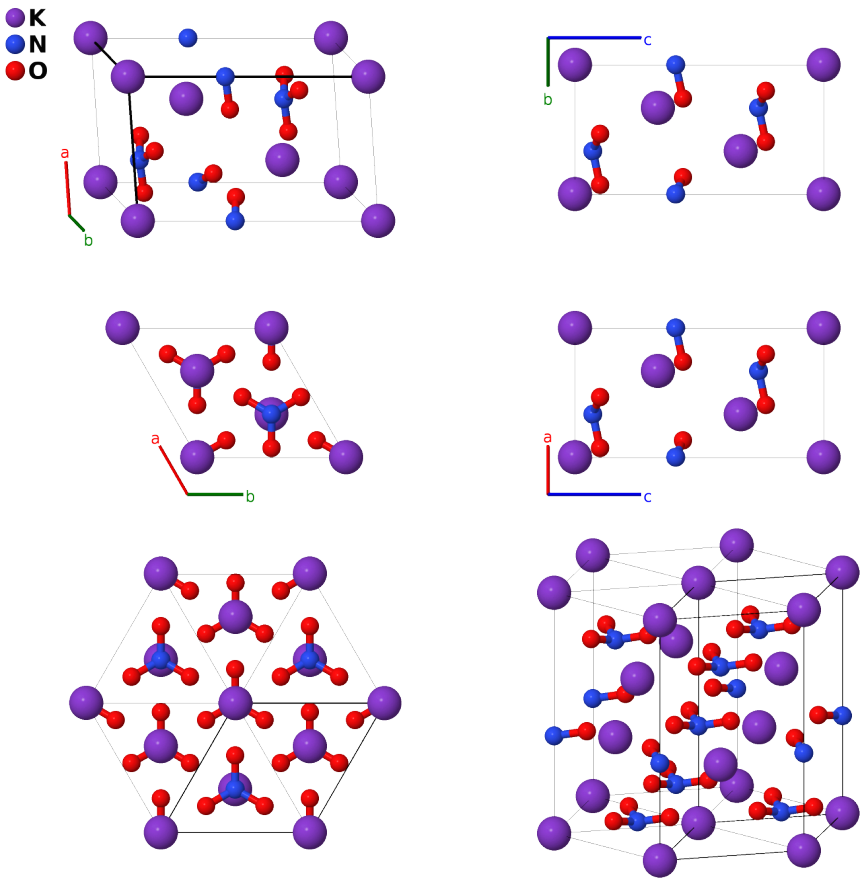
https://aflow.org/p/V4KY

https://aflow.org/p/ABC3_hR5_160_a_a_b-002



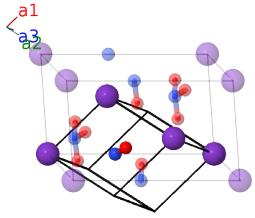
Prototype	KNO_3
AFLOW prototype label	ABC3_hR5_160_a_a_b-002
ICSD	384
Pearson symbol	hR5
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=ABC3_hR5_160_a_a_b-002 --params=`$a, c/a, x_1, x_2, x_3, z_3$

Other compounds with this structure
NH_4ClO_4, $BaTiO_3$

- 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.
- (Nimmo, 1976) give the data for γ-KNO_3 taken at 91°C.
- Although this is isostructural with the $KBrO_3$ ($G0_7$) structure, we have included it here to facilitate the comparison of the various KNO_3 phases.
- γ-KNO_3 and $KBrO_3$ ($G0_7$) have the same AFLOW prototype label, ABC3_hR5_160_a_a_b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings rhombohedral structures can be obtained with the option `--hex`.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(1a)	K I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(1a)	N I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_3 + z_3)\,\hat{\mathbf{z}}$	(3b)	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).