

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

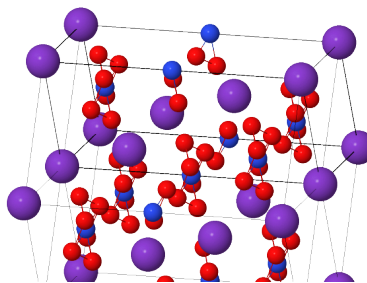
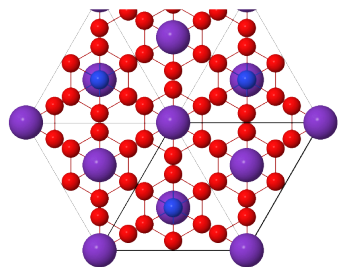
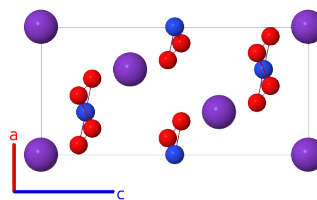
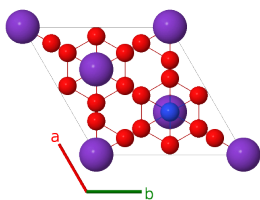
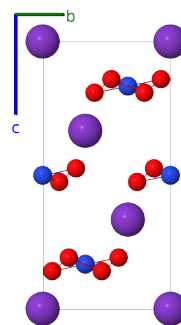
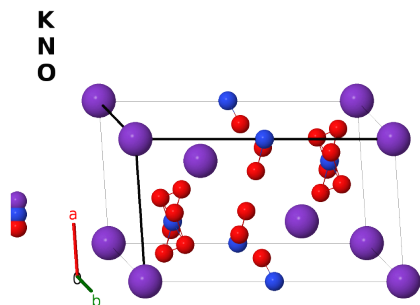
This structure previously used the label(s) **ABC6_hR8_166_a_b_h**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/XD6C>

https://aflow.org/prototype-encyclopedia/ABC6_hR8_166_a_b_h-001



Prototype	KNO_3
AFLOW prototype label	ABC6_hR8_166_a_b_h-001
ICSD	385

CCDC	1590914
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= $a, c/a, x_3, z_3$

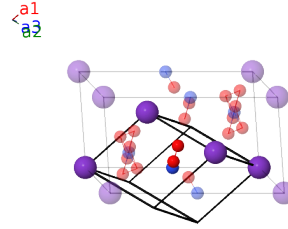
Other compounds with this structure

NaNO₃

- On heating, α -KNO₃ (either Structure I or Structure II) transforms into β -KNO₃ at 128°C. When heated above 200°C and then cooled, the β phase transforms into the metastable ferroelectric γ -KNO₃ 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

$$\begin{aligned}
 \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
 \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
 \end{aligned}$$



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).

First cited in

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.