# α-Potassium Nitrate (KNO$_3$) Structure I: ABC3_oP20_62_c_c_cd-001

This structure originally had the label `ABC3_oP20_62_c_c_cd.K.N.O3`. Calls to that address will be redirected here.

https://aflow.org/p/3DEN

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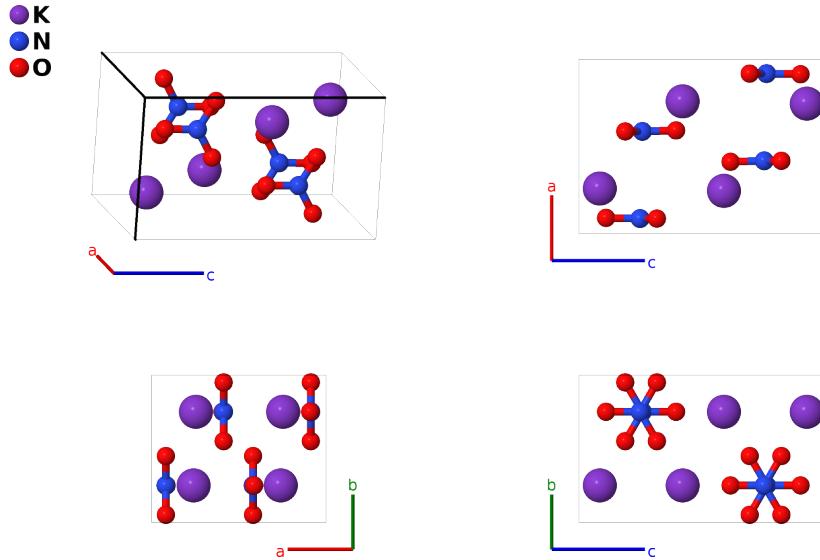
Prototype	KNO$_3$
AFLOW prototype label	ABC3_oP20_62_c_c_cd-001
ICSD	10289
Pearson symbol	oP20
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	`aflow --proto=ABC3_oP20_62_c_c_cd-001` `--params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

- Two possible structures have been identified for α-KNO$_3$: (Nimmo, 1973) proposed the current structure, which we call "Structure I," in space group $Pnma$ #62. (Adiwidjaja, 2003) found this structure, but also noted that it could be described by a doubling of the current unit cell into a superstructure with space group $Cmc2_1$ #36, which we call "Structure II". It is unclear to us which structure is correct, so we present both of them.

- (Nimmo, 1973) determined the lattice constants and Wyckoff positions of the type I structure at 25°C in the $Pmcn$ setting of space group #62. We present the data in the standard $Pnma$ setting.

- Argonite (CaCo$_3$, $G0_2$), α-KNO$_3$ I, and (NH$_4$)NO$_3$ III ($G0_{10}$) all share the same AFLOW label, ABC3_oP20_62_c_c_cd. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$
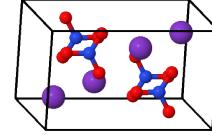
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_2}$	$=$	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_4}$	$=$	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	K I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	$=$	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_6}$	$=$	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	$=$	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_8}$	$=$	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	N I
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	$=$	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{10}}$	$=$	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a_1} + \frac{3}{4}\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	$=$	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	$=$	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a_1} + \frac{1}{4}\,\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{14}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a_1} - y_4\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{16}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{17}}$	$=$	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{18}}$	$=$	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a_1} + y_4\,\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	$=$	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{20}}$	$=$	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a_3}$	$=$	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II

References

[1] J. K. Nimmo and B. W. Lucas, *A neutron diffraction determination of the crystal structure of α-phase potassium nitrate at 25° C and 100° C*, J. Phys. C: Solid State Phys. **6**, 201–211 (1973), doi:10.1088/0022-3719/6/2/001.

[2] G. Adiwidjaja and D. Pohl, *Superstructure of α-phase potassium nitrate*, Acta Crystallogr. Sect. C **59**, i139–i140 (2003), doi:10.1107/S0108270103025277.

Found in

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