α-Potassium Nitrate (KNO_3) Structure II: ABC3_oC80_36_2ab_2ab_2a5b-001

This structure originally had the label `ABC3_oC80_36_2ab_2ab_2a5b`. Calls to that address will be redirected here.

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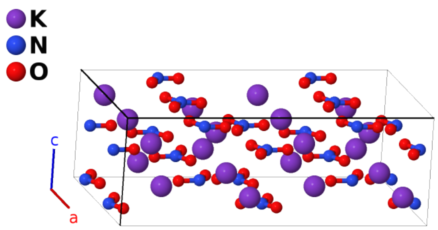
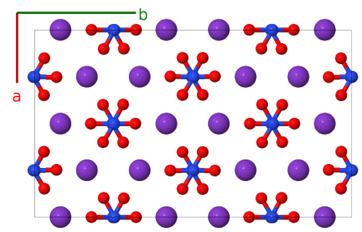
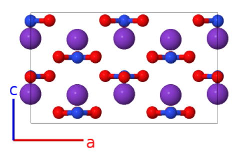
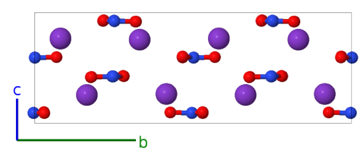
https://aflow.org/p/3YA6

https://aflow.org/p/ABC3_oC80_36_2ab_2ab_2a5b-001







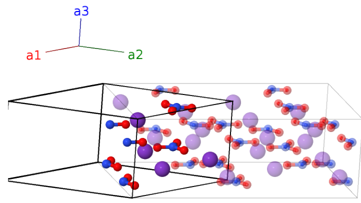


Prototype	KNO_3
AFLOW prototype label	ABC3_oC80_36_2ab_2ab_2a5b-001
ICSD	281552
Pearson symbol	oC80
Space group number	36
Space group symbol	$Cmc2_1$
AFLOW prototype command	`aflow --proto=ABC3_oC80_36_2ab_2ab_2a5b-001` `--params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}$

- Two possible structures have been identified for α-KNO_3: (Nimmo, 1973) proposed an orthorhombic structure in space group $Pnma$ #62, which we call "Structure I."
- (Adiwidjaja, 2003) found that structure, but also noted that it could be described by a doubling of the unit cell into a superstructure of type I, which we call "Structure II" and present on this page. It is unclear to us which structure is correct, so we present both. However, we do note that if we allow some uncertainity in the atoms of this structure, the findsym code shows it to be identical to Structure I.
- On heating, α-KNO_3 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 remains metastable at room temperature.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	K I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	K II
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	K II
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	N II
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	N II
$\mathbf{B_9}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{10}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{12}}$	=	$y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{13}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	K III
$\mathbf{B_{14}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	K III
$\mathbf{B_{15}}$	=	$(x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	K III
$\mathbf{B_{16}}$	=	$-(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8b)	K III
$\mathbf{B_{17}}$	=	$(x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8b)	N III
$\mathbf{B_{18}}$	=	$-(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	N III
$\mathbf{B_{19}}$	=	$(x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	N III
$\mathbf{B_{20}}$	=	$-(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8b)	N III
$\mathbf{B_{21}}$	=	$(x_9 - y_9)\,\mathbf{a}_1 + (x_9 + y_9)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8b)	O III
$\mathbf{B_{22}}$	=	$-(x_9 - y_9)\,\mathbf{a}_1 - (x_9 + y_9)\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8b)	O III

$\mathbf{B_{23}}$	=	$\left(x_{9}+y_{9}\right)\,\mathbf{a}_{1}+\left(x_{9}-y_{9}\right)\,\mathbf{a}_{2}+\left(z_{9}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{9}\,\mathbf{\hat{x}}-by_{9}\,\mathbf{\hat{y}}+c\left(z_{9}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{24}}$	=	$-\left(x_{9}+y_{9}\right)\,\mathbf{a}_{1}-\left(x_{9}-y_{9}\right)\,\mathbf{a}_{2}+z_{9}\,\mathbf{a}_{3}$	=	$-ax_{9}\,\mathbf{\hat{x}}+by_{9}\,\mathbf{\hat{y}}+cz_{9}\,\mathbf{\hat{z}}$	(8b)	O III
$\mathbf{B_{25}}$	=	$\left(x_{10}-y_{10}\right)\,\mathbf{a}_{1}+\left(x_{10}+y_{10}\right)\,\mathbf{a}_{2}+z_{10}\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}+by_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(8b)	O IV
$\mathbf{B_{26}}$	=	$-\left(x_{10}-y_{10}\right)\,\mathbf{a}_{1}-\left(x_{10}+y_{10}\right)\,\mathbf{a}_{2}+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}-by_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O IV
$\mathbf{B_{27}}$	=	$\left(x_{10}+y_{10}\right)\,\mathbf{a}_{1}+\left(x_{10}-y_{10}\right)\,\mathbf{a}_{2}+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{10}\,\mathbf{\hat{x}}-by_{10}\,\mathbf{\hat{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O IV
$\mathbf{B_{28}}$	=	$-\left(x_{10}+y_{10}\right)\,\mathbf{a}_{1}-\left(x_{10}-y_{10}\right)\,\mathbf{a}_{2}+z_{10}\,\mathbf{a}_{3}$	=	$-ax_{10}\,\mathbf{\hat{x}}+by_{10}\,\mathbf{\hat{y}}+cz_{10}\,\mathbf{\hat{z}}$	(8b)	O IV
$\mathbf{B_{29}}$	=	$\left(x_{11}-y_{11}\right)\,\mathbf{a}_{1}+\left(x_{11}+y_{11}\right)\,\mathbf{a}_{2}+z_{11}\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}+by_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{30}}$	=	$-\left(x_{11}-y_{11}\right)\,\mathbf{a}_{1}-\left(x_{11}+y_{11}\right)\,\mathbf{a}_{2}+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}-by_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{31}}$	=	$\left(x_{11}+y_{11}\right)\,\mathbf{a}_{1}+\left(x_{11}-y_{11}\right)\,\mathbf{a}_{2}+\left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{11}\,\mathbf{\hat{x}}-by_{11}\,\mathbf{\hat{y}}+c\left(z_{11}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{32}}$	=	$-\left(x_{11}+y_{11}\right)\,\mathbf{a}_{1}-\left(x_{11}-y_{11}\right)\,\mathbf{a}_{2}+z_{11}\,\mathbf{a}_{3}$	=	$-ax_{11}\,\mathbf{\hat{x}}+by_{11}\,\mathbf{\hat{y}}+cz_{11}\,\mathbf{\hat{z}}$	(8b)	O V
$\mathbf{B_{33}}$	=	$\left(x_{12}-y_{12}\right)\,\mathbf{a}_{1}+\left(x_{12}+y_{12}\right)\,\mathbf{a}_{2}+z_{12}\,\mathbf{a}_{3}$	=	$ax_{12}\,\mathbf{\hat{x}}+by_{12}\,\mathbf{\hat{y}}+cz_{12}\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{34}}$	=	$-\left(x_{12}-y_{12}\right)\,\mathbf{a}_{1}-\left(x_{12}+y_{12}\right)\,\mathbf{a}_{2}+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{12}\,\mathbf{\hat{x}}-by_{12}\,\mathbf{\hat{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{35}}$	=	$\left(x_{12}+y_{12}\right)\,\mathbf{a}_{1}+\left(x_{12}-y_{12}\right)\,\mathbf{a}_{2}+\left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{12}\,\mathbf{\hat{x}}-by_{12}\,\mathbf{\hat{y}}+c\left(z_{12}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{36}}$	=	$-\left(x_{12}+y_{12}\right)\,\mathbf{a}_{1}-\left(x_{12}-y_{12}\right)\,\mathbf{a}_{2}+z_{12}\,\mathbf{a}_{3}$	=	$-ax_{12}\,\mathbf{\hat{x}}+by_{12}\,\mathbf{\hat{y}}+cz_{12}\,\mathbf{\hat{z}}$	(8b)	O VI
$\mathbf{B_{37}}$	=	$\left(x_{13}-y_{13}\right)\,\mathbf{a}_{1}+\left(x_{13}+y_{13}\right)\,\mathbf{a}_{2}+z_{13}\,\mathbf{a}_{3}$	=	$ax_{13}\,\mathbf{\hat{x}}+by_{13}\,\mathbf{\hat{y}}+cz_{13}\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{38}}$	=	$-\left(x_{13}-y_{13}\right)\,\mathbf{a}_{1}-\left(x_{13}+y_{13}\right)\,\mathbf{a}_{2}+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$-ax_{13}\,\mathbf{\hat{x}}-by_{13}\,\mathbf{\hat{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{39}}$	=	$\left(x_{13}+y_{13}\right)\,\mathbf{a}_{1}+\left(x_{13}-y_{13}\right)\,\mathbf{a}_{2}+\left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_{3}$	=	$ax_{13}\,\mathbf{\hat{x}}-by_{13}\,\mathbf{\hat{y}}+c\left(z_{13}+\frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8b)	O VII
$\mathbf{B_{40}}$	=	$-\left(x_{13}+y_{13}\right)\,\mathbf{a}_{1}-\left(x_{13}-y_{13}\right)\,\mathbf{a}_{2}+z_{13}\,\mathbf{a}_{3}$	=	$-ax_{13}\,\mathbf{\hat{x}}+by_{13}\,\mathbf{\hat{y}}+cz_{13}\,\mathbf{\hat{z}}$	(8b)	O VII

References

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

[2] 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.