$RbNO_3$ (III) Structure: A8B24C_cP33_207_g_k_a-001

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https://aflow.org/prototype-encyclopedia/2SP7

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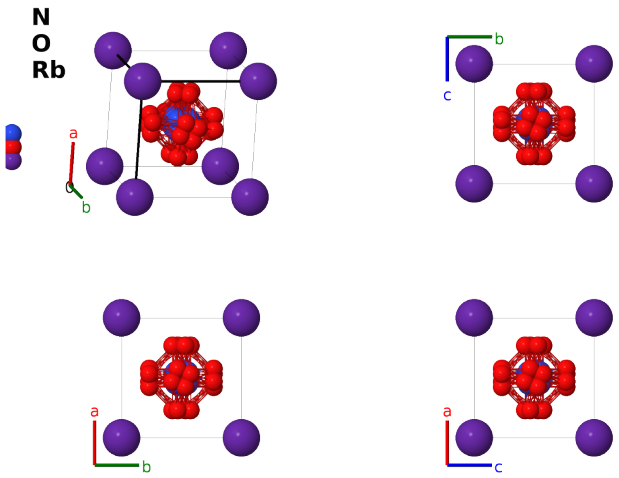


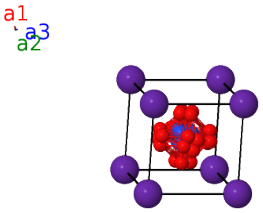
Prototype	NO_3Rb
AFLOW prototype label	A8B24C_cP33_207_g_k_a-001
ICSD	60966
CCDC	1624521
Pearson symbol	cP33
Space group number	207
Space group symbol	$P432$
AFLOW prototype command	`aflow --proto=A8B24C_cP33_207_g_k_a-001 --params=`a, x_2, x_3, y_3, z_3

- $RbNO_3$ takes on four distinct phases with increasing temperature (Shamsuzzoha, 1988):
  - Phase IV is the ground state, stable up to 437K.
  - Phase III, stable in the range 437-492K, is in this disordered cubic structure, where the NO_3 ions are centered on the halide site in the cesium chloride ($B2$) structure.
  - Phase II, stable up to 564K, is possibly a body-centered cubic structure with up to eight formula units in the conventional unit cell.
  - Phase I, stable up to the melting point, is thought to be a sodium chloride ($B1$) structure, with NO_3 again playing the role of chlorine.

- The nitrogen and oxygen sites are filled 12.5% of the time, so that only one nitrogen and three oxygens appear on any given halide site.
- Prior to 2023 this was the only ICSD entry for space group $P432$ #207.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Rb I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_9}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(8g)	N I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{12}}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{13}}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{14}}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{15}}$	=	$z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{16}}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{17}}$	=	$-z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{18}}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{19}}$	=	$-y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{20}}$	=	$y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{21}}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{22}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{23}}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{24}}$	=	$y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{25}}$	=	$-y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(24k)	O I

$\mathbf{B_{26}}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{27}}$	=	$-x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{28}}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{29}}$	=	$x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ay_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{30}}$	=	$z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{31}}$	=	$z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{32}}$	=	$-z_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(24k)	O I
$\mathbf{B_{33}}$	=	$-z_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(24k)	O I

References

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[2] M. Shamsuzzoha and B. W. Lucas, *Polymorphs of rubidium nitrate and their crystallographic relationships*, Canadian J. Chem. **66**, 819–823 (1988), doi:10.1139/v88-142.

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First cited in

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