

RbNO₃ (IV) Structure:

AB3C_hP45_144_3a_9a_3a-001

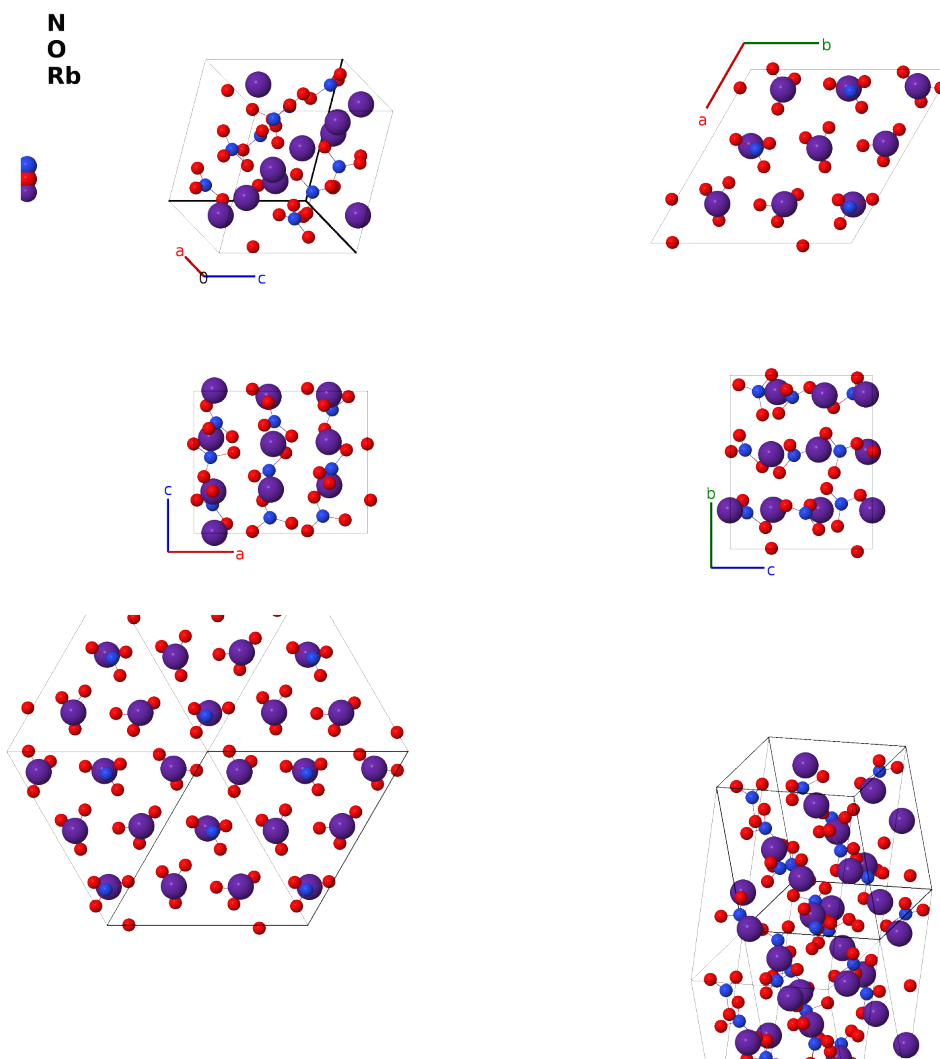
This structure previously used the label(s) **AB3C_hP45_144_3a_9a_3a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/UV9A>

https://aflow.org/prototype-encyclopedia/AB3C_hP45_144_3a_9a_3a-001



Prototype	NO ₃ Rb
AFLOW prototype label	AB3C_hP45_144_3a_9a_3a-001
ICSD	35102
CCDC	1607261

Pearson symbol	hP45
Space group number	144
Space group symbol	$P3_1$
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Other compounds with this structure

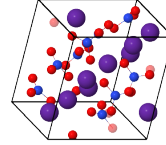
CsNO₃ (II), TiNO₃ (III)

- RbNO₃ takes on four distinct phases with increasing temperature (Shamsuzzoha, 1988):
 - Phase IV, presented here, is the ground state, stable up to 437K.
 - Phase III, stable in the range 437-492K, is in a disordered cubic structure, where the NO₃ 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 NO₃ again playing the role of chlorine.
- The phase IV structure also exists in the enantiomorphic space group $P3_2$ #145. (Shamsuzzoha, 1982)
- We used the data taken at room temperature, 298K.

Trigonal (Hexagonal) primitive vectors

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





Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= \frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(3a)	N I
$\mathbf{B}_2$	$-y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{3}) \mathbf{a}_3$	$= \frac{1}{2}a(x_1 - 2y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	N I
$\mathbf{B}_3$	$-(x_1 - y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{2}{3}) \mathbf{a}_3$	$= -\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + \frac{1}{3}c(3z_1 + 2) \hat{\mathbf{z}}$	(3a)	N I
$\mathbf{B}_4$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= \frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(3a)	N II
$\mathbf{B}_5$	$-y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{3}) \mathbf{a}_3$	$= \frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	N II
$\mathbf{B}_6$	$-(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{2}{3}) \mathbf{a}_3$	$= -\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + \frac{1}{3}c(3z_2 + 2) \hat{\mathbf{z}}$	(3a)	N II
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= \frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(3a)	N III

$\mathbf{B}_8 =$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	N III
$\mathbf{B}_9 =$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(3a)	N III
$\mathbf{B}_{10} =$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_{11} =$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_{12} =$	$-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(3a)	O I
$\mathbf{B}_{13} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_5 - y_5) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(3a)	O II
$\mathbf{B}_{14} =$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O II
$\mathbf{B}_{15} =$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + \frac{1}{3}c(3z_5 + 2) \hat{\mathbf{z}}$	(3a)	O II
$\mathbf{B}_{16} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_6 - y_6) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(3a)	O III
$\mathbf{B}_{17} =$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + (z_6 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O III
$\mathbf{B}_{18} =$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}} + \frac{1}{3}c(3z_6 + 2) \hat{\mathbf{z}}$	(3a)	O III
$\mathbf{B}_{19} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_7 - y_7) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(3a)	O IV
$\mathbf{B}_{20} =$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + (z_7 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O IV
$\mathbf{B}_{21} =$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + \frac{1}{3}c(3z_7 + 2) \hat{\mathbf{z}}$	(3a)	O IV
$\mathbf{B}_{22} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_8 - y_8) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(3a)	O V
$\mathbf{B}_{23} =$	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + (z_8 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O V
$\mathbf{B}_{24} =$	$-(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + \frac{1}{3}c(3z_8 + 2) \hat{\mathbf{z}}$	(3a)	O V
$\mathbf{B}_{25} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_9 - y_9) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(3a)	O VI
$\mathbf{B}_{26} =$	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + (z_9 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O VI
$\mathbf{B}_{27} =$	$-(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + (z_9 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + \frac{1}{3}c(3z_9 + 2) \hat{\mathbf{z}}$	(3a)	O VI
$\mathbf{B}_{28} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} + y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{10} - y_{10}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(3a)	O VII
$\mathbf{B}_{29} =$	$-y_{10} \mathbf{a}_1 + (x_{10} - y_{10}) \mathbf{a}_2 + (z_{10} + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{10} - 2y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O VII
$\mathbf{B}_{30} =$	$-(x_{10} - y_{10}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 + (z_{10} + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + \frac{1}{3}c(3z_{10} + 2) \hat{\mathbf{z}}$	(3a)	O VII
$\mathbf{B}_{31} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(3a)	O VIII
$\mathbf{B}_{32} =$	$-y_{11} \mathbf{a}_1 + (x_{11} - y_{11}) \mathbf{a}_2 + (z_{11} + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_{11} - 2y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{3}) \hat{\mathbf{z}}$	(3a)	O VIII
$\mathbf{B}_{33} =$	$-(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + (z_{11} + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + \frac{1}{3}c(3z_{11} + 2) \hat{\mathbf{z}}$	(3a)	O VIII

$$\begin{aligned}
\mathbf{B}_{34} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= \frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} + & (3a) & \text{O IX} \\
&&& cz_{12} \hat{\mathbf{z}} \\
\mathbf{B}_{35} &= -y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + &= \frac{1}{2}a(x_{12} - 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + & (3a) & \text{O IX} \\
&&& c(z_{12} + \frac{1}{3}) \hat{\mathbf{z}} \\
\mathbf{B}_{36} &= -(x_{12} - y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + &= -\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + & (3a) & \text{O IX} \\
&&& \frac{1}{3}c(3z_{12} + 2) \hat{\mathbf{z}} \\
\mathbf{B}_{37} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= \frac{1}{2}a(x_{13} + y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{13} - y_{13}) \hat{\mathbf{y}} + & (3a) & \text{Rb I} \\
&&& cz_{13} \hat{\mathbf{z}} \\
\mathbf{B}_{38} &= -y_{13} \mathbf{a}_1 + (x_{13} - y_{13}) \mathbf{a}_2 + &= \frac{1}{2}a(x_{13} - 2y_{13}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{13} \hat{\mathbf{y}} + & (3a) & \text{Rb I} \\
&&& c(z_{13} + \frac{1}{3}) \hat{\mathbf{z}} \\
\mathbf{B}_{39} &= -(x_{13} - y_{13}) \mathbf{a}_1 - x_{13} \mathbf{a}_2 + &= -\frac{1}{2}a(2x_{13} - y_{13}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{13} \hat{\mathbf{y}} + & (3a) & \text{Rb I} \\
&&& \frac{1}{3}c(3z_{13} + 2) \hat{\mathbf{z}} \\
\mathbf{B}_{40} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= \frac{1}{2}a(x_{14} + y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{14} - y_{14}) \hat{\mathbf{y}} + & (3a) & \text{Rb II} \\
&&& cz_{14} \hat{\mathbf{z}} \\
\mathbf{B}_{41} &= -y_{14} \mathbf{a}_1 + (x_{14} - y_{14}) \mathbf{a}_2 + &= \frac{1}{2}a(x_{14} - 2y_{14}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{14} \hat{\mathbf{y}} + & (3a) & \text{Rb II} \\
&&& c(z_{14} + \frac{1}{3}) \hat{\mathbf{z}} \\
\mathbf{B}_{42} &= -(x_{14} - y_{14}) \mathbf{a}_1 - x_{14} \mathbf{a}_2 + &= -\frac{1}{2}a(2x_{14} - y_{14}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{14} \hat{\mathbf{y}} + & (3a) & \text{Rb II} \\
&&& \frac{1}{3}c(3z_{14} + 2) \hat{\mathbf{z}} \\
\mathbf{B}_{43} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= \frac{1}{2}a(x_{15} + y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{15} - y_{15}) \hat{\mathbf{y}} + & (3a) & \text{Rb III} \\
&&& cz_{15} \hat{\mathbf{z}} \\
\mathbf{B}_{44} &= -y_{15} \mathbf{a}_1 + (x_{15} - y_{15}) \mathbf{a}_2 + &= \frac{1}{2}a(x_{15} - 2y_{15}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15} \hat{\mathbf{y}} + & (3a) & \text{Rb III} \\
&&& c(z_{15} + \frac{1}{3}) \hat{\mathbf{z}} \\
\mathbf{B}_{45} &= -(x_{15} - y_{15}) \mathbf{a}_1 - x_{15} \mathbf{a}_2 + &= -\frac{1}{2}a(2x_{15} - y_{15}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{15} \hat{\mathbf{y}} + & (3a) & \text{Rb III} \\
&&& \frac{1}{3}c(3z_{15} + 2) \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] M. Shamsuzzoha and B. W. Lucas, *Structure (neutron) of phase IV rubidium nitrate at 298 and 403 K*, Acta Crystallogr. Sect. B **38**, 2353–2357 (1982), doi:10.1107/S0567740882008772.
- [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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