# $RbNO_3$ (IV) Structure: AB3C_hP45_144_3a_9a_3a-001

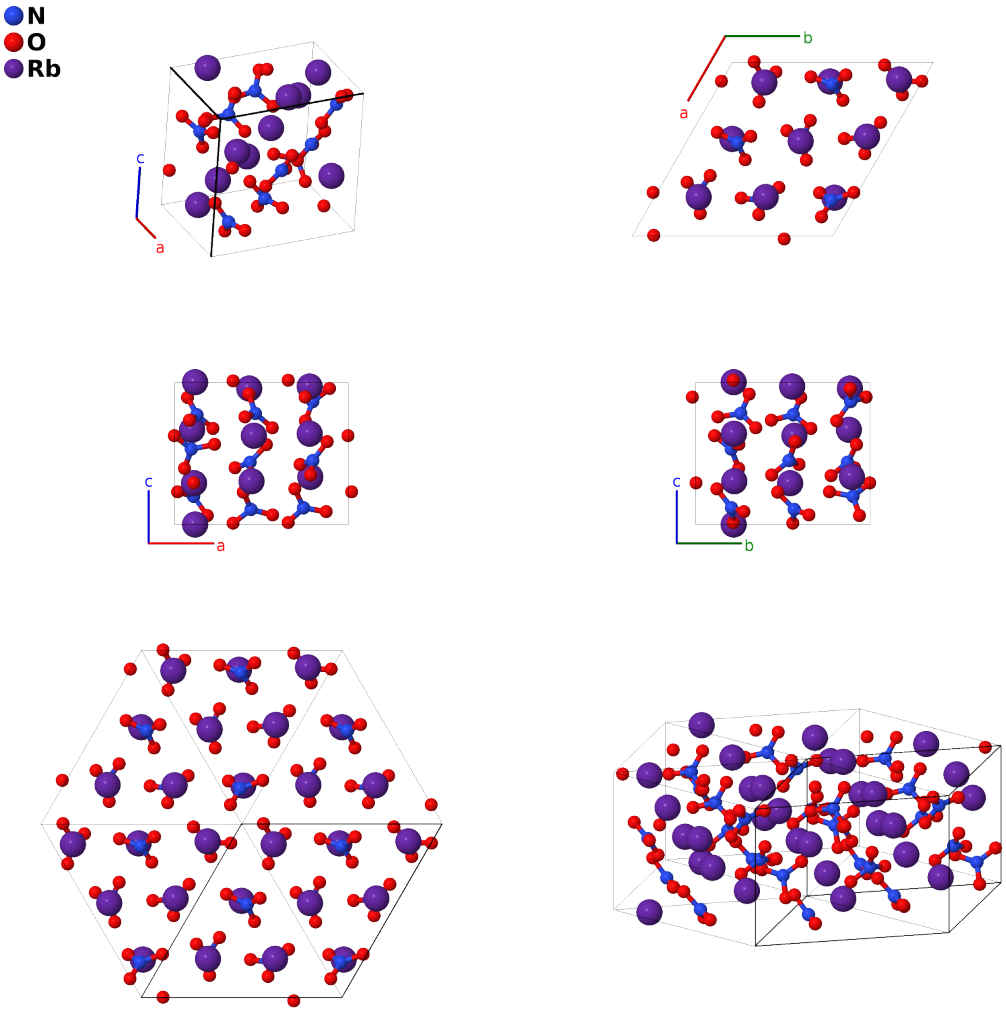
This structure originally had the label `AB3C_hP45_144_3a_9a_3a`. Calls to that address will be redirected here.

Cite this page as: 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.

---

https://aflow.org/p/UV9A

https://aflow.org/p/AB3C_hP45_144_3a_9a_3a-001




| | |
|---|---|
| **Prototype** | $NO_3Rb$ |
| **AFLOW prototype label** | AB3C_hP45_144_3a_9a_3a-001 |
| **ICSD** | 35102 |
| **Pearson symbol** | hP45 |
| **Space group number** | 144 |
| **Space group symbol** | $P3_1$ |

**AFLOW prototype command** `aflow --proto=AB3C_hP45_144_3a_9a_3a-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}$

---

**Other compounds with this structure**
$CsNO_3$ (II), $TlNO_3$ (III)

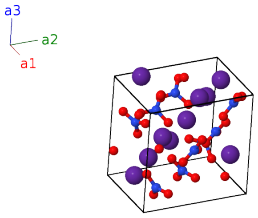
---

- $RbNO_3$ 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 the cesium chloride ($B2$) structure, with rubidium atoms on the cesium sites and orientationally disordered $NO_3$ ions on the chlorine sites.
  - 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 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**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$




---

**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 |
| $\mathbf{B_2}$ | = | $-y_1\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{3}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_1 - 2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{3}\right)\hat{\mathbf{z}}$ | (3a) | N I |
| $\mathbf{B_3}$ | = | $-(x_1 - y_1)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1 + \frac{2}{3}\right)\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_1 + 2)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_5}$ | = | $-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{3}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{3}\right)\hat{\mathbf{z}}$ | (3a) | N II |
| $\mathbf{B_6}$ | = | $-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{2}{3}\right)\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_2 + 2)\,\hat{\mathbf{z}}$ | (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 |
| $\mathbf{B_8}$ | = | $-y_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{3}\right)\mathbf{a}_3$ | = | $\frac{1}{2}a\,(x_3 - 2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{3}\right)\hat{\mathbf{z}}$ | (3a) | N III |
| $\mathbf{B_9}$ | = | $-(x_3 - y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{2}{3}\right)\mathbf{a}_3$ | = | $-\frac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3 + 2)\,\hat{\mathbf{z}}$ | (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 |

$$\mathbf{B_{11}} = -y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O I}$$

$$\mathbf{B_{12}} = -(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_4 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O I}$$

$$\mathbf{B_{13}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (3a) \quad \text{O II}$$

$$\mathbf{B_{14}} = -y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2 + \left(z_5 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O II}$$

$$\mathbf{B_{15}} = -(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_5 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O II}$$

$$\mathbf{B_{16}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (3a) \quad \text{O III}$$

$$\mathbf{B_{17}} = -y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O III}$$

$$\mathbf{B_{18}} = -(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_6 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O III}$$

$$\mathbf{B_{19}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IV}$$

$$\mathbf{B_{20}} = -y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IV}$$

$$\mathbf{B_{21}} = -(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(z_7 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_7 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IV}$$

$$\mathbf{B_{22}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8 + y_8)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_8 - y_8)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (3a) \quad \text{O V}$$

$$\mathbf{B_{23}} = -y_8\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_8 - 2y_8)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O V}$$

$$\mathbf{B_{24}} = -(x_8 - y_8)\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \left(z_8 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_8 - y_8)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_8 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O V}$$

$$\mathbf{B_{25}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_9 + y_9)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_9 - y_9)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VI}$$

$$\mathbf{B_{26}} = -y_9\,\mathbf{a}_1 + (x_9 - y_9)\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_9 - 2y_9)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VI}$$

$$\mathbf{B_{27}} = -(x_9 - y_9)\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_9 - y_9)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_9 + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VI}$$

$$\mathbf{B_{28}} = x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} + y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{10} - y_{10})\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VII}$$

$$\mathbf{B_{29}} = -y_{10}\,\mathbf{a}_1 + (x_{10} - y_{10})\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{10} - 2y_{10})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VII}$$

$$\mathbf{B_{30}} = -(x_{10} - y_{10})\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{10} - y_{10})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{10}\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_{10} + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VII}$$

$$\mathbf{B_{31}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11} + y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{11} - y_{11})\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VIII}$$

$$\mathbf{B_{32}} = -y_{11}\,\mathbf{a}_1 + (x_{11} - y_{11})\,\mathbf{a}_2 + \left(z_{11} + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{11} - 2y_{11})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VIII}$$

$$\mathbf{B_{33}} = -(x_{11} - y_{11})\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + \left(z_{11} + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{11} - y_{11})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{11}\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_{11} + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O VIII}$$

$$\mathbf{B_{34}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12} + y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_{12} - y_{12})\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IX}$$

$$\mathbf{B_{35}} = -y_{12}\,\mathbf{a}_1 + (x_{12} - y_{12})\,\mathbf{a}_2 + \left(z_{12} + \tfrac{1}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(x_{12} - 2y_{12})\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12} + \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IX}$$

$$\mathbf{B_{36}} = -(x_{12} - y_{12})\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + \left(z_{12} + \tfrac{2}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_{12} - y_{12})\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_{12}\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,(3z_{12} + 2)\,\hat{\mathbf{z}} \quad (3a) \quad \text{O IX}$$

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{37}}$ | $=$ | $x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{13}+y_{13})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{13}-y_{13})\;\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}}$ | (3a) | Rb I |
| $\mathbf{B_{38}}$ | $=$ | $-y_{13}\,\mathbf{a}_1 + (x_{13}-y_{13})\;\mathbf{a}_2 + \left(z_{13}+\frac{1}{3}\right)\;\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{13}-2y_{13})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{3}\right)\;\hat{\mathbf{z}}$ | (3a) | Rb I |
| $\mathbf{B_{39}}$ | $=$ | $-(x_{13}-y_{13})\;\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{2}{3}\right)\;\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_{13}-y_{13})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{13}\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_{13}+2)\;\hat{\mathbf{z}}$ | (3a) | Rb I |
| $\mathbf{B_{40}}$ | $=$ | $x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{14}+y_{14})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{14}-y_{14})\;\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}}$ | (3a) | Rb II |
| $\mathbf{B_{41}}$ | $=$ | $-y_{14}\,\mathbf{a}_1 + (x_{14}-y_{14})\;\mathbf{a}_2 + \left(z_{14}+\frac{1}{3}\right)\;\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{14}-2y_{14})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{1}{3}\right)\;\hat{\mathbf{z}}$ | (3a) | Rb II |
| $\mathbf{B_{42}}$ | $=$ | $-(x_{14}-y_{14})\;\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{2}{3}\right)\;\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_{14}-y_{14})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{14}\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_{14}+2)\;\hat{\mathbf{z}}$ | (3a) | Rb II |
| $\mathbf{B_{43}}$ | $=$ | $x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{15}+y_{15})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_{15}-y_{15})\;\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}}$ | (3a) | Rb III |
| $\mathbf{B_{44}}$ | $=$ | $-y_{15}\,\mathbf{a}_1 + (x_{15}-y_{15})\;\mathbf{a}_2 + \left(z_{15}+\frac{1}{3}\right)\;\mathbf{a}_3$ | $=$ | $\frac{1}{2}a\,(x_{15}-2y_{15})\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{3}\right)\;\hat{\mathbf{z}}$ | (3a) | Rb III |
| $\mathbf{B_{45}}$ | $=$ | $-(x_{15}-y_{15})\;\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{2}{3}\right)\;\mathbf{a}_3$ | $=$ | $-\frac{1}{2}a\,(2x_{15}-y_{15})\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{15}\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_{15}+2)\;\hat{\mathbf{z}}$ | (3a) | Rb III |

## 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 Journal of Chemistry **66**, 819–823 (1988), doi:10.1139/v88-142.