

Space group (207) *P432*207  
*cP33*

|                      |             |                         |
|----------------------|-------------|-------------------------|
| Rb[NO <sub>3</sub> ] | <i>cP33</i> | (207) <i>P432</i> – kgb |
|----------------------|-------------|-------------------------|

**RbNO<sub>3</sub> form III** [1]

Structural features: Rb atoms and NO<sub>3</sub> trigonal units (orientational disorder) in a CsCl-type arrangement.

Shamsuzzoha M., Lucas B.W. (1987) [1]

NO<sub>3</sub>Rb

$a = 0.44$  nm,  $V = 0.0852$  nm<sup>3</sup>,  $Z = 1$

| site | Wyck. | sym. | $x$           | $y$           | $z$           | occ.  | atomic environment |
|------|-------|------|---------------|---------------|---------------|-------|--------------------|
| O1   | $24k$ | 1    | 0.033         | 0.075         | 0.269         | 0.125 |                    |
| N2   | $8g$  | .3.  | 0.056         | 0.056         | 0.056         | 0.125 |                    |
| Rb3  | $1b$  | 432  | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |       |                    |

Transformation from published data:  $-x, -y, -z$ ; origin shift  $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, neutrons,  $wR = 0.061$ ,  $T = 461$  K

Remarks: Phase stable at  $437 < T < 492$  K. Short interatomic distances for partly occupied site(s). The present model was rejected in favor of a model with 12-fold orientational disorder of the nitrate groups in space group (221) *Pm-3m*.

References: [1] Shamsuzzoha M., Lucas B.W. (1987), Acta Crystallogr. C 43, 385-388.