

$\text{K}_5\text{Nb}_{11}[\text{Ge}_2\text{O}_7]\text{O}_{27}$  $hP106$  $(189) P-62m - 1^3_1 8_1 2^2_1 f^2 c$  **$\text{K}_{10}\text{Nb}_{22}\text{Ge}_4\text{O}_{68}$  [1]**

Structural features: Intergrowth of  $\text{Nb}_8\text{O}_{21}$  slabs (edge- and vertex-linked  $\text{NbO}_6$  octahedra) and  $\text{Nb}_6\text{Ge}_4\text{O}_{26}$  slabs (units of six vertex-linked  $\text{NbO}_6$  octahedra interconnected via common vertices with units of two vertex-linked  $\text{GeO}_4$  tetrahedra); K in channels perpendicular to [001] (partial disorder).

Choisnet J. et al. (1977) [1]

 $\text{Ge}_2\text{K}_5\text{Nb}_{11}\text{O}_{34}$  $a = 0.9112$ ,  $c = 2.001$  nm,  $c/a = 2.196$ ,  $V = 1.4388$  nm<sup>3</sup>,  $Z = 2$ 

| site | Wyck. | sym.        | $x$           | $y$           | $z$           | occ.  | atomic environment                    |
|------|-------|-------------|---------------|---------------|---------------|-------|---------------------------------------|
| O1   | 12l   | 1           | 0.182         | 0.502         | 0.291         |       | non-colinear Nb <sub>2</sub>          |
| O2   | 12l   | 1           | 0.206         | 0.483         | 0.133         |       | single atom Ge                        |
| O3   | 12l   | 1           | 0.313         | 0.491         | 0.408         |       | non-colinear Nb <sub>2</sub>          |
| O4   | 6i    | $\bar{3}m$  | 0.179         | 0             | 0.394         |       | non-colinear Nb <sub>2</sub>          |
| O5   | 6i    | $\bar{3}m$  | 0.202         | 0             | 0.19          |       | non-colinear Nb <sub>2</sub>          |
| Nb6  | 6i    | $\bar{3}m$  | 0.234         | 0             | 0.097         |       | octahedron O <sub>6</sub>             |
| Nb7  | 6i    | $\bar{3}m$  | 0.251         | 0             | 0.285         |       | octahedron O <sub>6</sub>             |
| K8   | 6i    | $\bar{3}m$  | 0.598         | 0             | 0.203         | 0.833 | 12-vertex polyhedron O <sub>12</sub>  |
| Nb9  | 6i    | $\bar{3}m$  | 0.744         | 0             | 0.41          |       | octahedron O <sub>6</sub>             |
| O10  | 6i    | $\bar{3}m$  | 0.795         | 0             | 0.307         |       | non-coplanar triangle Nb <sub>3</sub> |
| O11  | 6i    | $\bar{3}m$  | 0.799         | 0             | 0.088         |       | non-colinear Nb <sub>2</sub>          |
| Ge12 | 4h    | 3 $\bar{2}$ | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.09          |       | tetrahedron O <sub>4</sub>            |
| Nb13 | 4h    | 3 $\bar{2}$ | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.351         |       | octahedron O <sub>6</sub>             |
| K14  | 3g    | $m2m$       | 0.344         | 0             | $\frac{1}{2}$ | 0.833 | 4-vertex polyhedron O <sub>4</sub>    |
| O15  | 3g    | $m2m$       | 0.79          | 0             | $\frac{1}{2}$ |       | non-colinear Nb <sub>2</sub>          |
| O16  | 3f    | $m2m$       | 0.252         | 0             | 0             |       | non-colinear Nb <sub>2</sub>          |
| K17  | 3f    | $m2m$       | 0.547         | 0             | 0             | 0.833 | trigonal bipyramid O <sub>5</sub>     |
| O18  | 2c    | $\bar{6}..$ | $\frac{1}{3}$ | $\frac{2}{3}$ | 0             |       | colinear Ge <sub>2</sub>              |

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ Experimental: powder, diffractometer, X-rays,  $R_B = 0.080$ 

References: [1] Choynet J., Hervieu M., Groult D., Raveau B. (1977), Mater. Res. Bull. 12, 621-627.