

$\text{K}_3\text{Nb}_6[\text{VO}_4]\text{O}_{15}$  $hP116$  $(189) P-62m - 1^3 1^9 h^3 g^2 f^2 e$ **K<sub>3</sub>Nb<sub>6</sub>VO<sub>19</sub>** [1]

Structural features: Intergrowth of Nb<sub>8</sub>O<sub>21</sub> slabs (edge- and vertex-linked NbO<sub>6</sub> octahedra) and Nb<sub>6</sub>V<sub>4</sub>O<sub>30</sub> slabs (units of six vertex-linked NbO<sub>6</sub> octahedra interconnected via common vertices with VO<sub>4</sub> tetrahedra).

Haddad A., Jouini T. (1996) [1]

 $\text{K}_3\text{Nb}_6\text{O}_{19}\text{V}$  $a = 0.9114$ ,  $c = 2.4044$  nm,  $c/a = 2.638$ ,  $V = 1.7296$  nm<sup>3</sup>,  $Z = 4$ 

| site | Wyck. | sym.       | $x$           | $y$           | $z$           | occ. | atomic environment                    |
|------|-------|------------|---------------|---------------|---------------|------|---------------------------------------|
| O1   | 12l   | 1          | 0.1696        | 0.482         | 0.4212        |      | non-colinear Nb <sub>2</sub>          |
| O2   | 12l   | 1          | 0.1746        | 0.4773        | 0.0924        |      | non-colinear VNb                      |
| O3   | 12l   | 1          | 0.316         | 0.4828        | 0.324         |      | non-colinear Nb <sub>2</sub>          |
| O4   | 6i    | $\bar{3}m$ | 0.1772        | 0             | 0.1595        |      | non-colinear Nb <sub>2</sub>          |
| O5   | 6i    | $\bar{3}m$ | 0.208         | 0             | 0.3392        |      | non-coplanar triangle Nb <sub>3</sub> |
| Nb6  | 6i    | $\bar{3}m$ | 0.2321        | 0             | 0.0783        |      | octahedron O <sub>6</sub>             |
| Nb7  | 6i    | $\bar{3}m$ | 0.2518        | 0             | 0.4222        |      | octahedron O <sub>6</sub>             |
| K8   | 6i    | $\bar{3}m$ | 0.4055        | 0             | 0.2414        |      | 10-vertex polyhedron O <sub>10</sub>  |
| Nb9  | 6i    | $\bar{3}m$ | 0.7553        | 0             | 0.325         |      | octahedron O <sub>6</sub>             |
| O10  | 6i    | $\bar{3}m$ | 0.8017        | 0             | 0.4099        |      | non-coplanar triangle Nb <sub>3</sub> |
| O11  | 6i    | $\bar{3}m$ | 0.8221        | 0             | 0.2525        |      | non-colinear Nb <sub>2</sub>          |
| O12  | 6i    | $\bar{3}m$ | 0.8235        | 0             | 0.0661        |      | non-colinear Nb <sub>2</sub>          |
| V13  | 4h    | 3..        | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.1184        |      | tetrahedron O <sub>4</sub>            |
| O14  | 4h    | 3..        | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.1854        |      | single atom V                         |
| Nb15 | 4h    | 3..        | $\frac{1}{3}$ | $\frac{2}{3}$ | 0.3695        |      | octahedron O <sub>6</sub>             |
| O16  | 3g    | $m2m$      | 0.2083        | 0             | $\frac{1}{2}$ |      | non-colinear Nb <sub>2</sub>          |
| K17  | 3g    | $m2m$      | 0.5953        | 0             | $\frac{1}{2}$ |      | trigonal prism O <sub>6</sub>         |
| O18  | 3f    | $m2m$      | 0.2881        | 0             | 0             |      | non-colinear Nb <sub>2</sub>          |
| K19  | 3f    | $m2m$      | 0.583         | 0             | 0             |      | coplanar triangle O <sub>3</sub>      |
| Nb20 | 2e    | 3.m        | 0             | 0             | 0.1985        |      | octahedron O <sub>6</sub>             |

Transformation from published data: origin shift 0 0  $\frac{1}{2}$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.031, T = 293 K

References: [1] Haddad A., Jouini T. (1996), J. Solid State Chem. 124, 244-249.