

$K_{10}Ga_3Sb_{6.33}$  $hP40$  $(176) P6_3/m - h^6cb$ **K<sub>20</sub>Ga<sub>6</sub>Sb<sub>12.66</sub>** [1]

Structural features: Infinite columns of base-linked GaK<sub>6</sub>Sb<sub>3</sub>, SbK<sub>6</sub>(Ga<sub>2</sub>K) and SbK<sub>6</sub>(GaK<sub>2</sub>) tricapped trigonal prisms share atoms to form a 3D-framework with AlB<sub>2</sub>-type (BaLiSi) columns (9 prisms in the triangular cross-section); additional Sb in channels of hexagonal section parallel to [001] (partial disorder). Planar Ga<sub>3</sub>Sb<sub>6</sub> units formed by three vertex-linked GaSb<sub>3</sub> trigonal units (a Ga<sub>3</sub>Sb<sub>3</sub> ring with an additional Sb bonded to each Ga). Ordering variant of Ce<sub>2</sub>NiSi.

Cordier G., Ochmann H. (1990) [1]

 $Ga_3K_{10}Sb_{6.33}$  $a = 1.78$ ,  $c = 0.5438$  nm,  $c/a = 0.306$ ,  $V = 1.4921$  nm<sup>3</sup>,  $Z = 2$ 

| site | Wyck. | sym.  | $x$    | $y$    | $z$   | occ. | atomic environment   |
|------|-------|-------|--------|--------|-------|------|--|
| K1   | 6h    | $m..$ | 0.0065 | 0.1942 | $1/4$ |      | square pyramid Sb <sub>5</sub>   |
| K2   | 6h    | $m..$ | 0.0645 | 0.452  | $1/4$ |      | 15-vertex polyhedron Sb <sub>5</sub> Ga <sub>2</sub> K <sub>8</sub>      |
| K3   | 6h    | $m..$ | 0.2732 | 0.3931 | $1/4$ |      | 15-vertex polyhedron Sb <sub>5</sub> Ga <sub>2</sub> K <sub>8</sub>      |
| Sb4  | 6h    | $m..$ | 0.3414 | 0.2275 | $1/4$ |      | single atom Ga   |
| Ga5  | 6h    | $m..$ | 0.5036 | 0.28   | $1/4$ |      | coplanar triangle Sb <sub>3</sub>  |
| Sb6  | 6h    | $m..$ | 0.5514 | 0.1627 | $1/4$ |      | non-colinear Ga <sub>2</sub>   |
| K7   | 2c    | -6..  | $1/3$  | $2/3$  | $1/4$ |      | sixcapped hexagonal prism Ga <sub>6</sub> Sb <sub>6</sub> K <sub>6</sub> |
| Sb8  | 2b    | -3..  | 0      | 0      | 0     | 0.33 | square prism (cube) Sb <sub>2</sub> K <sub>6</sub>                       |

Transformation from published data:  $y, x, -z$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.090

Remarks: In [1] the number of formula units per cell Z is misprinted as 4 instead of 1.

References: [1] Cordier G., Ochmann H. (1990), Z. Naturforsch. B 45, 277-282.