Crystal structure of potassium niobate, \( \text{K}_6\text{Nb}_{10.80}\text{O}_{30} \), a partially filled tetragonal tungsten bronze-type structure

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Abstract

\( \text{K}_6\text{Nb}_{10.80}\text{O}_{30} \), tetragonal, \( P4/mmb \) (No. 127), \( a = 12.537(2) \text{ Å}, c = 3.9730(1) \text{ Å}, V = 624.5 \text{ Å}^3, Z = 1, R_{\text{st}}(F) = 0.037, wR_{\text{ref}}F^2 = 0.119, T = 293 \text{ K}. \)

Source of material

The title compound was prepared in the course of a systematic investigation of the ternary system \( \text{K}_2\text{O}-\text{Nb}_2\text{O}_5-\text{B}_2\text{O}_3 \). It crystallizes within a wide range of ternary composition: 20 mol% < \( x(\text{K}_2\text{O}) \) < 35 mol%, 8 mol% < \( x(\text{B}_2\text{O}_3) \) < 50 mol%, 22 mol% < \( x(\text{Nb}_2\text{O}_5) \) < 55 mol%, but does not occur in the binary system \( \text{K}_2\text{O}-\text{Nb}_2\text{O}_5 \). \( \text{K}_6\text{Nb}_{10.80}\text{O}_{30} \) was grown from a melt with molar composition of \( \text{Nb}_2\text{O}_5: \text{K}_2\text{CO}_3: \text{B}_2\text{O}_3 \) of 1:0.857:1 to colorless, long-prismatic crystals which were separated from the flux using hot diluted hydrochloric acid.

Table 2. Atomic coordinates and displacement parameters (in Å²).

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<th>( y )</th>
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* Correspondence author (e-mail: p.held@kri.uni-koeln.de)
Table 2. Continued.

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References