

Redetermination of the structure of $\text{PNb}_9\text{O}_{25}$

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Description

Nonaniobium phosphorus pentacosaoxide, $\text{PNb}_9\text{O}_{25}$, $M_r = 1267.11$, tetragonal, $I4/m$, $a = 15.639$ (2), $c = 3.8317$ (4) Å, $V = 937.1$ (3) Å³, $Z = 2$, $D_x = 4.49$ Mg m⁻³, $A(\text{Mo K}\alpha) = 0.71073$ Å, $\mu(\text{Mo K}\alpha) = 5.27$ mm⁻¹, $F(000) = 584$, $T = 294$ K, 316 reflections with $I > 3\sigma(I)$, $R = 0.033$, $wR = 0.031$. The framework is composed of ReO_3 -type $3 \times 3 \times 3$ columns. Each column shares edges with the four neighboring columns and corners with the PO_4 tetrahedra.

Experimental. During the study of the K-Nb-PO system single crystals of $\text{PNb}_9\text{O}_{25}$ were isolated. The crystal structure of this compound had already been determined by Roth, Wadsley & Anderson (1965) using integrated Weissenberg photographs. However, the R factor remained rather high (0.093), some atoms had negative thermal factors and some problems remain with the choice of the space group. So we performed a new data collection on an automatic diffractometer in ...