Interpenetrierende Clusterstränge in
der Kristallstruktur von K_{0.77}Nb_6Cl_{15}

Interpenetrating Cluster Chains in
the Structure of K_{0.77}Nb_6Cl_{15}

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The solid state reaction of KCl, NbCl\textsubscript{5} and Nb powder at 760 °C yielded black crystals of KNb\textsubscript{6}Cl\textsubscript{15}. The structure of the compound has been determined using single-crystal X-ray methods. KNb\textsubscript{6}Cl\textsubscript{15} crystallizes in the orthorhombic space group \textit{Pnma} (no. 51) with lattice constants \(a = 1780.1(2), b = 1341.4(1), \) and \(c = 925.5(1)\) pm, \(Z = 4, \) and \(R1 = 0.039\) for all 2727 observed reflections.

\[\text{[(Nb}_{6}\text{Cl}_{12}^\text{i})\text{Cl}_{6}^{2\text{-}\text{a-a}}]\text{–}\text{ anions in the structure are linked via two Cl}^{\text{a-a}}\text{ bridges to form one set of linear and one set of kinked chains along the crystallographic } c \text{ and } a \text{ directions. Four remaining Cl}^{\text{a-a}}\text{ bridges interconnect both sets of chains to a three-dimensional network. The potassium occupancy on a } 4k \text{ site was refined to a value of } 0.384(3) \text{ consistent with the formula } \text{K}_{0.77}\text{Nb}_6\text{Cl}_{15}.\]