The Crystal Structure of NbO_2I – A Double-layer Structure with 7-Coordinated Niobium

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Single crystals of NbO_2I were obtained as dark red needles by chemical transport. According to the structure determination (*Pnma*, $a = 20.897(4)$, $b = 3.7654(8)$, $c = 3.9715(8)$ Å, $Z = 4$, 619 reflections, 26 variables, $R_1(F) = 0.0645$, $wR_2(F^2) = 0.1597$) NbO_2I represents a new structure type with 7-coordinated Nb atoms. Pentagonal bipyramids NbO_5I_2 are connected *via* the apical O atoms with alternating short and long Nb–O distances (1.79 / 2.20 Å) to chains and *via* the three equatorial O atoms to double layers. Between the double layers there are only weak van-der-Waals interactions of the I atoms. NbO_2I is the first oxide halide of a transition metal with CN 7. Structurally NbO_2I is closely related to UO_2Br, but with alternating short and long Nb–O distances as a difference.

Key words: Niobium Oxide Halide, Double-layer Structure, 7-Coordination, Single Crystal, Structure Determination