

Ein neues Selten-Erd-Metall(III)-Oxidchlorid-Oxotellurat(IV): $\text{Nd}_5\text{O}_4\text{Cl}_3[\text{TeO}_3]_2$

A New Rare Earth-Metal(III) Oxide Chloride Oxotellurate(IV): $\text{Nd}_5\text{O}_4\text{Cl}_3[\text{TeO}_3]_2$

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Pale violet, plate-like single crystals of the title compound, neodymium(III) oxide chloride oxotellurate(IV) $\text{Nd}_5\text{O}_4\text{Cl}_3[\text{TeO}_3]_2$, can be obtained by the reaction of Nd_2O_3 with NdCl_3 and TeO_2 in equimolar ratios in evacuated silica ampoules within five days at 775 °C with an excess of CsCl added as fluxing agent. $\text{Nd}_5\text{O}_4\text{Cl}_3[\text{TeO}_3]_2$ crystallizes in the monoclinic space group $C2/m$ (no. 12) with the lattice parameters $a = 1270.61(9)$, $b = 562.70(4)$, $c = 1008.97(8)$ pm, $\beta = 90.784(3)^\circ$ and $Z = 2$, and is thus isostructural to the lanthanoid(III) oxide halide oxoselenates(IV) $\text{Tb}_5\text{O}_4\text{Cl}_3[\text{SeO}_3]_2$ and $\text{Gd}_5\text{O}_4\text{Br}_3[\text{SeO}_3]_2$. The crystal structure exhibits three crystallographically different Nd^{3+} cations, of which $(\text{Nd}1)^{3+}$ has a purely oxidic coordination sphere of eight oxide anions building up a square prism. $(\text{Nd}2)^{3+}$ and $(\text{Nd}3)^{3+}$ are both coordinated by oxide and chloride anions. The coordination polyhedron around $(\text{Nd}2)^{3+}$ is a trigonal prism of oxide anions that is capped by one chloride anion to give a coordination number of seven. $(\text{Nd}3)^{3+}$ resides in an eightfold coordination of five oxide and three chloride anions forming a square antiprism. All $(\text{O}1)^{2-}$ anions are surrounded tetrahedrally by Nd^{3+} cations as $[\text{ONd}_4]^{10+}$ units. These tetrahedra share common edges and vertices to generate two-dimensional infinite layers of the composition $\overset{2}{\infty}\{[\text{O}_4\text{Nd}_5]^{7+}\}$, which extend parallel to the (001) plane. The chloride anions $(\text{Cl}1)^-$ are connecting those slabs *via* $\text{Nd}3\text{--Cl}1\text{--Nd}3$ bridges along the [001] direction, while the $(\text{Cl}2)^-$ anions alternate with the Te^{4+} cations above and below the layers. The three-dimensional crystal structure of $\text{Nd}_5\text{O}_4\text{Cl}_3[\text{TeO}_3]_2$ is completed by Te^{4+} cations, which are bonded to one $(\text{O}2)^{2-}$ and two $(\text{O}3)^{2-}$ anions to form ψ^1 -tetrahedra $[\text{TeO}_3]^{2-}$ with a *non-binding*, stereochemically active electron pair (“lone pair”) pointing into the free space between the chloride-decorated $\overset{2}{\infty}\{[\text{O}_4\text{Nd}_5]^{7+}\}$ layers.

Key words: Neodymium, Oxide, Chloride, Oxotellurate(IV), Crystal Structure