

MS15-P1 Crystal structure features of christofschäferite-(Ce) a new mineral of chevkinite-group. Sergey M. Aksenov,^a Ramiza K. Rastsvetaeva,^a Nikita V. Chukanov,^b ^aShubnikov Institute of Crystallography, Russia, ^bInstitute of Problems of Physical Chemistry, Russia
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The crystal structure of a new species of chevkinite-group minerals christofschäferite-(Ce) from the Eifel Mountains, Rhineland-Palatinate, Germany was studied by X-ray single crystal diffraction (diffractometer Xcalibur Oxford Diffraction with CCD-detector). The monoclinic unit-cell parameters are: $a = 13.3722(4)$ Å, $b = 5.7434(1)$ Å, $c = 11.0862(2)$ Å, $\beta = 100.580(2)^\circ$, $V = 836.97(4)$ Å³, space group: $P2_1/m$. The structure was solved by direct methods and refined to $R=5.5$, $4560F > 3\sigma_F$.

The crystal structure of christofschäferite-(Ce) is similar to that of other chevkinite-group minerals. Sheets of small and distorted Ti-centred octahedra (with minor admixtures of Fe³⁺, Al and Nb) lie parallel to the (100) plane. These sheets are interleaved with a layer consisting of Si₂O₇ groups and larger M1O₆ octahedra with a mean cation-anion distance of 2.188 Å. REE and subordinate Ca occupy the sites A1 – A4 with coordination numbers from 8 to 10. The rare earth ions lie in the channels of the structure framework.

Based on the interatomic distances and bond valence calculations, we consider the following occupancy of octahedral sites:

M1 – Mn²⁺ with subordinate Fe²⁺; M2, M2' and M3 – Ti with subordinate Fe³⁺, Fe²⁺ and minor Nb; M4 – Fe³⁺, Fe²⁺ and Ti with mean charge about +3.

The site M1 with the mean cation-anion distance of 2.188 Å and the mean charge close to 2 is the only site that can contain Mn²⁺. The crystal-chemical formula of christofschäferite-(Ce), taking into account chemical data, is $X(\text{Ce}, \text{REE}, \text{Ca})_2 \text{VIII}(\text{Ce}, \text{REE}, \text{Ca})_2 \text{VI}(\text{Mn}, \text{Fe}^{2+}) \text{VI}(\text{Ti}, \text{Fe}, \text{Al})_4 (\text{Si}_2\text{O}_7)_2\text{O}_8$.

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Keywords: X-ray analysis; mineral; silicate

MS15-P2 Crystal Structure of the Fluorite-like Nd₅Mo₃O₁₆ Compound. Olga Alekseeva,^a Natalya Sorokina,^a Igor Verin,^a Nadezhda Bolotina,^a Anna Gagor,^b Adam Pietraszko,^b Elena Kharitonova,^c Valentina Voronkova,^c ^aShubnikov Institute of Crystallography RAS, Russia, ^bTrzebiatowski Institute of Low Temperature and Structure Research PAS, Poland, ^cMoscow State University, Russia
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High oxygen conductivity (0.06 Sm/cm at 800°C) of the La₂Mo₂O₉ compound (1:2) was established in the La₂O₃ – MoO₃ system by the Lacorre et al [1]. There is no such a compound in the Nd₂O₃ - MoO₃ system, but there is one with the fluorite-like structure near the Nd₂MoO₆. The phase formation in the Nd₂O₃ - MoO₃ (25 - 50 mol.% Nd₂O₃) system was previously studied in details [2]. It was confirmed that the composition of this compound might be different due to its existence in the 43 - 47 mol.% Nd₂O₃ homogeneity area. The Nd₅Mo₃O₁₆ single crystals were grown within the same work. Their mixed electronic-ionic conductivity has been revealed, with air-conduction electron component not exceeding 10% [3]. In the present work the unit-cell values of the Nd₅Mo₃O₁₆ single crystal were measured in temperature range from 295K to 30K, and its structure was studied using the X-rays diffraction technique at 293K, 110K and 30K temperatures. The unit-cell values were always cubic relating to that of CaF₂ fluorite as $a \approx 2a_f$ ($a_f = 5.5$ Å). The structure was solved within the P n3 n symmetry group. It was found that all the atoms are disordered over several positions, with the most significantly disordered Nd₂, Mo, O₂ atoms. The MoO₄-tetrahedra in the Nd₅Mo₃O₁₆ structure have no common vertices or faces. Each of them is a separate and sufficiently free fragment of the structure, which is able to move from its main crystallographic position due to its interaction with the neodymium atoms. An indirect confirmation for the violation of translational periodicity in the distribution of Mo and Nd atoms was obtained. Thus, it was found that the Nd₅Mo₃O₁₆ compound has a disordered fluorite-like structure. It was shown that the oxidation state of molybdenum atoms in this structure is less than +6, which explains the appearance of the electronic component of conductivity. The ionic conductivity of Nd₅Mo₃O₁₆ compound is associated with the disordering of the oxygen atoms by several positions, and their deficiency in comparison with the initial fluorite.

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