

Cs₃NdSi₈O₁₉ und Cs₆Nd₂Si₂₁O₄₈:

Zwei cäsiumhaltige Oxosilicate des Neodyms im Vergleich

Cs₃NdSi₈O₁₉ and Cs₆Nd₂Si₂₁O₄₈: Two Caesium-containing Oxosilicates of Neodymium in Comparison

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Z. Naturforsch. **2009**, 64b, 1329–1338; received Oktober 10, 2009

Professor Hubert Schmidbaur zum 75. Geburtstag gewidmet

In the quaternary system Cs / Nd / Si / O, two new representatives, the *phyllo*-oxosilicate Cs₃NdSi₈O₁₉ and the *tecto*-oxosilicate Cs₆Nd₂Si₂₁O₄₈, were synthesized by CsF-flux-supported solid-state reactions between Nd₂O₃ and SiO₂. The first one, Cs₃NdSi₈O₁₉ (orthorhombic, *Cmcm* (no. 63), *a* = 705.74(5), *b* = 2712.85(19), *c* = 1163.72(8) pm, *Z* = 4), is not isotypic to the related scandium compound Cs₃ScSi₈O₁₉. The [SiO₄]⁴⁻ tetrahedra (*d*(Si⁴⁺–O²⁻) = 156–163 pm) in the structure of Cs₃NdSi₈O₁₉ are connected *via* common corners to form corrugated, loop-branched double layers containing four- and eight-membered rings in the (010) plane and eight-membered rings along [001]. Each of the eight-membered ellipses emerging along [100] is additionally loop-branched by two four-membered chains. The oxosilicate double layers are cross-linked by vertex-sharing *via* otherwise isolated [NdO₆]⁹⁻ octahedra (*d*(Nd³⁺–O²⁻) = 232–234 pm) to build up a three-dimensional framework. Also in between the oxosilicate double layers, the (Cs1)⁺ cations are located on the 8*f* site. Each of the octagonal channels along [001] hosts one (Cs3)⁺ and two (Cs2)⁺ cations, which both reside at only partially occupied sites (8*g* and 8*f*, respectively) and disorder, because otherwise too short Cs⁺...Cs⁺ distances would occur. The second compound, Cs₆Nd₂Si₂₁O₄₈, crystallizes also in an orthorhombic space group (*Pmmn* (no. 59), *a* = 2189.24(15), *b* = 731.92(5), *c* = 1593.61(11) pm, *Z* = 2). Starting from a loop-branched single layer containing five- and eight-membered rings, a three-dimensional framework of vertex-shared [SiO₄]⁴⁻ tetrahedra (*d*(Si⁴⁺–O²⁻) = 149–164 pm) built up, in which the Si–O distances range from 149 to 164 pm within a broad range. In certain cavities, one kind of Nd³⁺, but four kinds of Cs⁺ cations (here, all sites with full occupation) are embedded. Also surrounded by only six O²⁻ anions just like in the first case, the Nd³⁺ cations (*d*(Nd³⁺–O²⁻) = 233–237 pm) exhibit an unusually small, but not unknown coordination sphere for this relatively large lanthanoid(III) cation.

Key words: Neodymium, Oxosilicates, Caesium, Crystal Structures