Quaternäre Strontium-Kupfer(I)-Lanthanoid(III)-Selenide mit Cer und Praseodym: $SrCuCeSe_3$ und $SrCuPrSe_3$, ein ungleiches Geschwisterpaar

Quaternary Strontium Copper(I) Lanthanoid(III) Selenides with Cerium and Praseodymium: $SrCuCeSe_3$ and $SrCuPrSe_3$, Unequal Brother and Sister

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Quaternary strontium copper(I) lanthanoid(III) selenides are formed by the oxidation of elemental strontium, copper and the corresponding lanthanoid with selenium. Orange to red needle-shaped single crystals of $SrCuPrSe_3$ and $SrCuCeSe_3$ have been synthesized by heating mixtures of Sr, Cu, Pr / Ce and Se with CsI as a flux in evacuated silica tubes to 800 °C for 7 d. Both compounds crystallize orthorhombically in space group *Pnma* with four formula units per unit cell, but with unlike lattice constants ($a = 1097.32(6)$, $b = 416.51(2)$, $c = 1349.64(8)$ pm for $SrCuPrSe_3$ and $a = 846.13(5)$, $b = 421.69(2)$, $c = 1663.42(9)$ pm for $SrCuCeSe_3$) and therefore different structure types. The Pr^{3+} cations in $SrCuPrSe_3$ are surrounded octahedrally by six Se^{2-} anions forming chains of edge-sharing $[PrSe_6]^{9-}$ octahedra that are joined by common vertices. Together with $[CuSe_4]^{7-}$ tetrahedra they form $[CuPrSe_3]^{2-}$ layers piled up parallel (001). Between those layers the Sr^{2+} cations are coordinated by seven Se^{2-} anions in the shape of capped trigonal prisms linking the structure in the third dimension. On the other hand in $SrCuCeSe_3$ the Ce^{3+} cations as well as the Sr^{2+} cations adopt a coordination number of seven. Since the bonding distances between cerium and selenium match with those of strontium and selenium the two crystallographically independent sites of these cations are occupied statistically by Ce^{3+} and Sr^{2+} with equal ratios. Nevertheless, there is a close structural relationship between $SrCuPrSe_3$ and $SrCuCeSe_3$. Similar to $SrCuPrSe_3$ where Cu^{+} and Pr^{3+} cations together with Se^{2-} anions form $[CuPrSe_3]^{2-}$ layers parallel (001), the Cu^{+} cations and $[(Ce1/Sr1)Se_7]^{11.5-}$ polyhedra in $SrCuCeSe_3$ build strongly puckered layers which are connected by $(Ce2)^{3+}/(Sr2)^{2+}$ cations. The copper selenium part in both compounds correlates as well, with $[CuSe_4]^{7-}$ tetrahedra linked by common vertices to form $[CuSe_3]^{5-}$ chains running along [010].

Key words: Lanthanides, Copper, Strontium, Selenides, Crystal Structures