New Intermetallic Compounds forming the $Ca_{11}Ga_7$ Structure Type

Caroline Röhr, Marco Wendorff, *Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany*. E-mail: caroline@ruby.chemie.uni-freiburg.de

The binary alkaline earth (A^{II}) trielides $Ca_{11}Ga_7$ [1] and $Sr_{11}In_7$ [2] crystallize with a singular structure type (cubic, space group *Fm3m*, *a* ≈ 1620 (A=Ca)/1750 pm (A=Sr)). Fourteen new ternary Ca and Sr trielides (M^{III})/tetrelides (M^{IV}) forming this structure type were synthesized from stoichiometric mixtures of the elements and characterized by single crystal x-ray diffraction. The structures exhibit isolated M(1) atoms (M(1)=Al, Ga, In, Sn, Pb) together with tetrahedral units $[M(2)_4]$, which are formed by the triel elements exclusively. Remarkably, one of the four crystallographically independent A^{II} positions is – as in the pure element – coordinated by A partners of the same kind in a cuboctahedral arrangement. In the mixed M^{III}/M^{IV} compounds, the phase range reaches up to a maximum composition limit of $A_{11}[M(1)^{III}_4][M(2)^{IV}]_3$, which nearly corresponds to a ionic description according to the Zintl concept (tetrahedral anions $[M^{III}_4]^{8-}$ isoelectronic to white phosphorus P_4 besides isolated noble gas isosteric anions $[M^{IV}]^{3-}$). In the case of the Sr/In/Pb compounds, even the Sr position coordinated by Sr only is substituted by Pb^{4-}. The stabilities and phase ranges of the compounds, which are influenced by geometric and electronic factors (investigated by FP-LAPW band structure calculations) will be discussed.

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