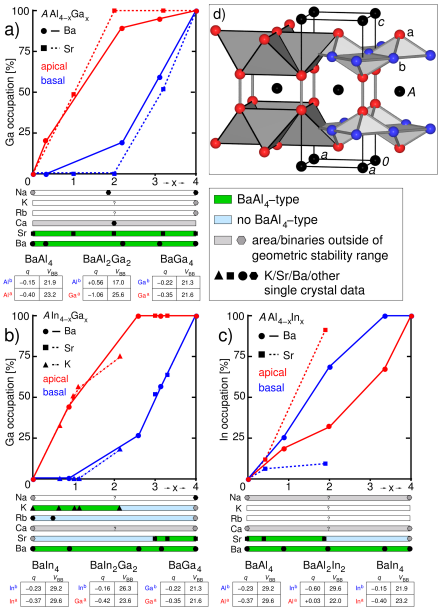

Figure 1. Triel-distribution in ternary compounds (investigated by means of single crystal data, black symbols) of the series $AAl_{4-x}Ga_x$ (a), $AIn_{4-x}Ga_x$ (b), $AAl_{4-x}In_x$ (c) forming the $BaAl_4$-type structure (d).

Keywords: Trielides, Gallides, Indides, Aluminides, Synthesis, Bandstructure Calculation

MS15-P4 Twinning and pseudosymmetry in $CsLan_2F$ compounds with cation arrays equivalent to the hexagonal Laves phase Zn_2Mg

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Ternary rare earth fluorides are of interest for a wide range of optical applications like e.g. lasers, scintillators, luminescent materials or efficient up- and downconverters e.g. [1]. The understanding and interpretation of their optical properties relies on an unambiguous structure determination. However, structure determination is frequently difficult due to the occurrence of complex twinning. One of the underlying reasons for this is the close relationship of the materials to high symmetry structures like fluoride, pyrochlore or tveitite [2-4].

Surprisingly ternary fluorides with general composition $ALan_2F_7$ with A=K,Rb,Cs and Lan=rare earths and Y have been described in a large variety of different space groups, although the main structural motifs are very similar. It is also striking that for many of the described structures discussions about the correct space groups are ongoing.

We have investigated the compounds $CsLan_2F_7$ with Lan=Nd,Gd,Tb,Er,Yb,Lu and Y with single crystal x-ray diffraction using synchrotron radiation. All the compounds show a pseudo-hexagonal metrics with $a \approx b \approx 15.5\text{-}16.5$ Å, $c \approx 12.3\text{-}12.7$ Å and $\gamma \approx 120°$. A detailed analysis of the data shows that the structures are best described in the monoclinic space group $P112_1/b$ taking into account additional six-fold twinning. To better understand the underlying reasons for the frequent occurrence of twinning in the samples we performed a detailed analysis of the pseudosymmetry of the crystal structures, which showed that, in particular the cation array has a very high pseudosymmetry with respect to space group $P6_3/mmc$ with lattice parameter $a_{hex} = 1/2a$, $c_{hex} = c$. Surprisingly, the resulting cation array in this high symmetry structure shows atomic positions which are equivalent to the ones observed in the hexagonal Laves phases Zn_2Mg. An analysis of the pseudosymmetry of the structures of the known $ALan_2F_7$ compounds shows the same highly symmetrical cation array.

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Keywords: ternary fluorides; twinning; pseudosymmetry; Laves phases