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Structural investigations of mixed anionic rare-earth and transition metals selenide oxides using synchrotron radiation

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The simultaneous reaction of oxygen, its heavier homologs, and metals usually lead to the formation of substances characterized by the presence of covalent O-*Ch* (*Ch* = S, Se) bonds within complex anions like sulfates or selenides. Examples for compounds containing both, O^{2-} and Ch^{2-} without any attractive interaction between these species are far less known. Only a few examples for chalcogenide oxides of transition (*T*) and rare-earth metals (*RE*) are described in the literature so far, though exhibiting a relatively high variety in composition and crystal structures.
Salt-flux assisted reactions of rare-earth metals and their oxides, transition metals and selenium lead to the discovery of the mixed anionic selenide oxides $RE_2ZrSe_2O_3$ (*RE* = Ce-Nd, Sm) and $Ce_7TiSe_5O_7$. All these substances appear as thin needle-like crystals with diameters of 5 µm and less which are extraordinarily sensitive to mechanical stress. Consequently, structure determination had to be realized using synchrotron radiation. First investigations of $Ce_7TiSe_5O_7$ were carried out at the ESRF, beamline ID11, using micro-focused synchrotron radiation. Small crystals were pre-selected and pre-characterized using transmission electron microscopy including EDX spectroscopy [1]. The substance crystallizes with the $La_7VSe_5O_7$ structure type [2], space group *Cmcm*, suggesting the presence of Ti^{3+} cations.
The first Zr containing selenide oxides $RE_2ZrSe_2O_3$ (= 2 $RE^{3+}Zr^{4+}2Se^{2-}3O^{2-}$) were investigated at PETRA III, beamline P24, and the ESRF, beamline ID11. The compounds were found to crystallize with their own structure type, space group $C\,2/m$, characterized by the presence of large cavities extended along [010] formed by Se atoms (see Fig. 1).

Fig. 1: a-c) Crystal structure, bulk material, and SEM-SE image of $Nd_2ZrSe_2O_3$. d) TEM-BF image of the $Pr_2ZrSe_2O_3$ single-crystal investigated at ERSF, beamline ID11. The crystal part used for structure determination is emphasized.

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[2] S. Peschke, L. Gamperl, V. Weippert, D. Johrendt, Dalton Trans. 2017, 46, 6230-6243.

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