

MS15-P10 Crystal structures of NaLnF₄ (Ln = La, Ce, Pr, Nd, Sm, and Gd) studied with synchrotron single-crystal and powder diffraction. Andrzej Grzechnik,^a Karen Friese,^b ^aInstitute of Crystallography, RWTH Aachen University, Germany, ^bJülich Centre for Neutron Science, Germany
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The most efficient host material for green and blue up-conversion known to date is hexagonal NaYF₄ doped with lanthanides [1]. It is used in optical fibers, solar cells, and immunoassay detectors. Different synthesis methods and up-conversion processes in the colloidal, bulk, and nanocrystalline materials have been extensively studied over last decades. The high efficiency of the up-conversion in the NaXF₄ compounds (X=rare earth or Y) is related to the multisite character of their crystal structure. The average structure of the NaXF₄ compounds at room temperature, i.e., of the β polymorphs, is described in space group P $\bar{6}$ [2]. In addition, layers of diffuse scattering, which are related to partial ordering of the cations, are observed [2]. The β phases with Y and heavier rare earths transform to the fluorite-type a structure (space group Fmm) at 900-1000 K [3]. The cubic a phases are characterized by complete cationic disorder.

Here we present our structural investigations of the NaLnF₄ compounds (Ln = La, Ce, Pr, Nd, Sm, and Gd) at ambient and high pressures using synchrotron radiation. The single-crystal datasets for Ln = La, Ce, Nd, Sm, and Gd measured at ambient pressure can be indexed with unit cells of $a \sim 6.1$ Å and $c \sim 3.8$ Å (space group P $\bar{6}$) [2]. However, weak superstructure reflections are observed in the single-crystal dataset for NaPrF₄. They can be indexed with a large unit cell $a = 10.617(1)$ Å and $c = 7.499(5)$ Å (space group P3). The structural model could be derived on the basis of group-subgroup relationships. This superstructure is due to further partial ordering of the Na⁺ and Pr³⁺ cations as well as of vacancies. Our observations suggest that the b structure is unstable and that the ordering is a slow process at ambient conditions that eventually affects the optical properties of these materials.

The high-pressure studies using synchrotron powder and single-crystal diffraction in diamond anvil cells at room temperature demonstrate that β -NaNdF₄ and β -NaGdF₄ as well as the superstructure NaPrF₄ are stable on compression to at least 8 GPa with no evidence for any pressure-induced order-disorder phenomena. The hexagonal metrics of the b-NaLnF₄ compounds at ambient conditions can be converted into a pseudocubic one using the relationships $a_{\text{cubic}} = 1/3a_{\text{hex}} - 1/3b_{\text{hex}} + 2/3c_{\text{hex}}$, $b_{\text{cubic}} = 1/3a_{\text{hex}} + 2/3b_{\text{hex}} + 2/3c_{\text{hex}}$, $c_{\text{cubic}} = -2/3a_{\text{hex}} - 1/3b_{\text{hex}} + 2/3c_{\text{hex}}$. The deviations from the cubic metrics are minimal for the average structure of NaPrF₄ and only at high pressures, a significant deviation is observed. For NaGdF₄, the deviations from the cubic metrics get smaller at higher pressures.

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MS15-P11 Mineralogical composition of atmospheric dust in Pilsen studied by X-ray powder diffraction. David Havlicek,^a Jiri Plocek^b, Miroslav Klan^c, ^aDept. of Inorg. Chem., ^aFaculty of Science, Charles University in Prague, Albertov 6, 128 43 Praha 2, Czech Republic, ^bInst. of Inorg. Chem. of the ASCR, v.v.i., Husinec – Rez 1001, 250 68 Rez u Prahy, Czech Republic, ^cEnvironmental Department, Municipality of Pilsen, Kopeckého sady 10, 306 32 Czech Republic
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Our work deals with the study of mineralogical composition of solid fraction of ambient aerosol in Pilsen basin, and its source apportionment. Our technology consists of collection dust particles on glass fibre (non-diffracting) filters in different paces around the city and at different meteorological conditions. The filters were worked up by X-ray powder diffraction using parallel-beam geometry and by electron microscopy. The origin of dust and source apportionment was studied with use of direct mineralogical analysis of potential dust sources (transport – engines, tyres, brakes, local burning places, heat plants ashes, building industry, quarries etc.) by X-ray diffraction. The minerals significant for each source were identified and searched on filters collecting atmospheric dust. As one result, the appearance of actinolite fibres on filters and localisation of its source in stones used for pavement, coming from neighbouring quarry, led to the closure of that quarry.

Keywords: atmospheric dust; mineralogical composition; X-ray powder diffraction; parallel beam technique