Structure of the hydrated phase of RbD₂PO₄ (DRDP) : RbD₂PO₄*₅D₂O. S. Mattauch¹, W. Paulus², J. Glinnemann³ and G. Heger⁴. "Inst. f. Kristallographie, RWTH Aachen; ²LCSIM Université Rennes I.

RbH₂PO₄ (RDP) and RbD₂PO₄ (DRDP) are known for a long time and belonging to the Hydrogen/Deuterium bonded ferroelectric. The best known representative of this family is KDP. In order to get a better understanding of the polymorphism of the KDP-family, especially with respect to the role of the hydrogen bonds and the H/D isotope effect, we have started a program focussed on the Rb- and Tl-compounds. The existence of the hydrated phase RbD₂PO₄*₅D₂O was already mentioned by A. V. Mishenko et al. as early as 1972, but no information on the crystals structure with its lattice and spacegroup was given. By X-ray and neutron diffraction we were able to prove the existence of the mono-hydrate phase, the detailed crystal structure analysis of which is presented in the paper.

Electrostatic bonds between the Rubidium atom and the PO₄ tetrahedra with respect to the fully ordered deuterium structure analysis of which is presented in the paper.

For growing the single crystals of RbD₂PO₄*₅D₂O the standard procedure for DRDP was used:

\[ Rb₂(CO₃)₂ + 2D₂PO₄ \xrightarrow{} 2RbD₂PO₄ + CO₂ + D₂O \]

Depending on the history of the solution DRDP or RbD₂PO₄*₅D₂O crystals are obtained. Under a closed atmosphere which prevents also an exchange of D⇌H the crystals are stable at room temperature. The structure was determined by combined neutron (S2 ORPHEE Reactor, CE Saclay) and X-ray (Stoe IPDS) single crystal investigations at room temperature. The unitcell was found to be monoclinic with:

\[ P \perp 2_1/c \]
\[ a = 7.262(1) Å, b = 7.466(1) Å, c = 9.481(1) Å, \]
\[ \beta = 104.91(1), V = 515.36 Å³ \]
\[ Z = 4 \]

The structure consists of double layers of PO₄ tetrahedra with respect to the fully ordered deuterium bonding. The double layers them self are linked by electrostatic bonds between the Rubidium atom and the PO₄ tetrahedrons. In between this double layer structure lies a D₂O plane, linked by a hydrogen bonds to the double layers.

Under heating RbD₂PO₄*₅D₂O dehydrates below 329(5)K and undergoes a reconstructive phase transition to DRDP.

Lifetime of small Ni⁺⁺⁺⁺-Polarons in Sr₀.₆₁Ba₀.₃₉Nb₂O₆:Ce,Cr and KNbO₃. Th. Woike¹, D. Berben¹,², M. Imlau¹, K. Buse³, R. Pankrath², E. Krätzig². "Institut für Kristallographie, Universität zu Köln, Zülpicherstr. 49b, 50674 Köln, Germany, ²Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany.

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The existence of small polarons in Niobate-crystals is of importance for both holographic data storage and frequency conversion such as second harmonic generation.

If doped single crystals of LiNbO₃, KNbO₃ or Sr₀.₆₁Ba₀.₃₉Nb₂O₆ are illuminated with continuous light or short laser pulses with sufficiently high intensity in the visible spectral range, electrons are excited into the conduction band. These electrons can be trapped by Nb⁵⁺⁻ ions. The coulomb-interaction of a trapped electron distorts the crystal lattice, thus lowering the potential energy of the electron. The electron is now trapped inside its own potential hole. Because this localized state is only weakly bound, these polarons decay at room temperature after short lifetimes. However, they show an extremely broad absorption band. Its maximum lies in the near-infrared region, and it may extend well into the visible spectral range. This light-induced absorption can seriously influence second harmonic generation and holographic data storage.

We show the temperature-dependence of the lifetime and the non-exponential decay of small polarons in Cerium resp. Chromium-doped SBN and nominally pure KNbO₃ after excitation with a short laser pulse of λ=532 nm. Further illumination with a pulse of λ=1064 nm after a delay of about 10 ns does not destroy the polarons, but causes a charge-transport. This mechanism is sensitive to the distance between the polaron and the next possible trapping-center. The result of this distance-dependent charge-transport is a polaron-hopping. With absorption spectra we show the influence of light-induced polaron-absorption on second harmonic generation.

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