5<sup>th</sup> International Workshop on 11-132 DYNAMICS IN CONFINEMENT Oct

Contribution ID: 16

Type: Oral

## Factors governing ferroelectric ordering of water molecules confined in beryl

Wednesday, 12 October 2022 16:20 (20 minutes)

Beryl crystals contain structural voids which may be partly occupied by single molecules of water. Due to the local symmetry of the atoms around the voids, the molecules experience sets of potential minima with respect to their angular orientations. The molecules remain fairly independent of the neutral crystal lattice, and they are mutually separated by several Å. Thus, they cannot interconnect by hydrogen bonds, and the dipole-dipole interaction is dominant. In partly hydrated beryl, the water molecules tend to order directionally on cooling. In fact, dielectric spectroscopy has revealed a ferroelectric-like soft phonon in the far-infrared region. However, no ferroelectric ordering appeared, the soft-phonon frequency leveling off below ~10 K. This was explained by quantum fluctuations occurring at low temperatures.

In order to gain a deeper insight into the ordering mechanisms, we conducted a theoretical study by mean-field approximation and Monte Carlo simulations. These have shown that in an ideal ground state, the dipoles are aligned ferroelectrically in the ab planes and antiferroelectrically in the c direction. This order is suppressed by quantum tunneling, as well as by the disorder in the hydration (empty voids).

Using NMR spectroscopy, we studied the molecules' positional geometry and their dynamical behavior. Up to now, it was assumed that in equilibrium, the H-H lines are parallel to the c crystal axis. In contrast, the measured NMR spectra clearly indicate that the H–H lines deviate from the c axis by ~18°. Most probably, the molecules form O–H-O hydrogen bonds with an oxygen atoms near the void. We propose that the O atoms stay in place while the H atoms perform twofold movements: (i) occasional jumps among the 12 possible binding O sites in the void, and (ii) oscillations around the O-H-O bonds. The frequency of the oscillations, as evaluated from our thermodynamic analysis, agrees well with an earlier published theoretical model.

**Primary authors:** Dr KADLEC, Filip (Institute of Physics, Czech Academy of Sciences); Dr CHLAN, Vojtěch (Faculty of Mathematics and Physics, Charles University); Mr ADAMEC, Martin (Institute of Physics, Czech Academy of Sciences); Prof. JANIŠ, Václav (Institute of Physics, Czech Academy of Sciences); Dr ANTONÍN, Klíč (Institute of Physics, Czech Academy of Sciences)

Presenter: Dr KADLEC, Filip (Institute of Physics, Czech Academy of Sciences)

Session Classification: Talks

Track Classification: Contributions