Contribution ID: **73** Type: **Poster**

Role of water molecules in the phase transitions in lawsonite

Wednesday, 9 September 2020 15:50 (30 minutes)

Lawsonite [CaAl2Si2O7(OH)2·H2O] is an uncommon mineral found in metamorphic rocks, occurring at subduction zones, supposedly at depths of up to 250 km. It contains 11.5 wt% water in its crystal structure. At room temperature, it is orthorhombic, crystallizing in the Cmcm space group. Its structure contains a silicate tetrahedra framework with four formulas in the unit cell. Each chemical formula comprises one water molecule embedded in a structural cavity; these cavities form channels parallel with the c axis. The protons form O-H bonds, and they may diffuse along the channels. The static and dynamic orientations of the water molecules plays a key role in two low-temperature phase transitions—a structural one at 270 K, and a ferroelectric one at 124 K. We studied the lattice dynamics in a single crystal of lawsonite using infrared, Raman and THz time-domain spectroscopies. We have found a strong soft phonon mode linked to the ferroelectric phase transition. The observed unusual hardening of other phonons with heating is linked to anomalous temperature dependence of a unit cell parameter. In view of a dielectric anomaly identified earlier, our results show that the ferroelectric phase transition is of mixed displacive / order-disorder type.

Presenter: KADLEC F. (Institute of Physics, Academy of Sciences of the Czech Republic, Prague)

Session Classification: Poster session