



Foreign molecules and ions in beryl obtained by infrared and visible spectroscopy

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Beryl minerals of Serbia were slightly studied in the last century and despite that there is some obtainable data about main characteristics there is a limited amount of information about foreign molecules in the mineral structure.

Two beryl samples from different locations in Serbia were examined in detail but infrared spectroscopy (IR) and spectrophotometry (VIS) was used for determination of foreign molecules and ions in the structure and the obtained data is shown in this paper.

The infrared (IR) and visible spectra (VIS) of two natural beryl samples indicate the presence of two types of water molecule, Fe²⁺, Fe³⁺ ions and CO₃. The spectra of two types of water molecules can be recognized with molecular fundamental vibrations at 3687 cm⁻¹ (asymmetric stretching) for type I, at 3574 cm⁻¹ and 3585 cm⁻¹ both symmetric stretching, and with deformation vibrations at 1627 cm⁻¹ and 1632 cm⁻¹ for type II. In range of symmetric stretching there is broad vibrational band which can be explained by presence of water molecules type II near alkali ions. Overtones and combinations of these fundamental vibrations have been identified. The type I molecules have their C₂ symmetry axes perpendicular to the crystal C₆ axis, while the type II molecules are rotated by 90 degrees and have their C₂ symmetry axes parallel to the crystal C₆ axis. Vibrational absorption frequency of 1425 cm⁻¹ indicate the presence of CO₃. Pale blue beryl is colored according to the relative intensities of two spectral features attributable to iron ions: a) a broad band in the extraordinary ray (Er) at 16000 cm⁻¹ due to Fe²⁺ in a channel site and b) a broad band in range of 22500-31400 cm⁻¹ in both ordinary ray (Or) and Er due to octahedral Fe³⁺ in the Al³⁺ site. Two other features, also attributable to iron, do not produce any visible coloration: a) an absorption edge at 12350 cm⁻¹ in Or is due to Fe²⁺ in the octahedral site and b) a broad band in Er and Or, centered around 12350 cm⁻¹, is due to Fe²⁺ in channel site. These spectral features are interpreted on the basis of the crystal field theory.

Infrared and visible spectroscopy data of two natural beryl minerals from Serbia has shown that water molecules, carbonates and iron ions represent the main impurities in the crystal structure. Nature of the fluid inclusions and quantitative content of Fe²⁺ and Fe³⁺ ions remain to be examined in the future.