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A POLARIZED SINGLE-CRYSTAL STUDY OF SYNTHETIC WATER-POOR BERYL

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Beryl typically contains extraframework alkali-ions, H_2O and/or CO_2 molecules in the structural channel. The water molecules occur in two different orientations: type I , having their two-fold axis perpendicular to the *c* axis of beryl, and type II, typically adjacent to alkali ions, having their two-fold symmetry axis parallel to [100] (e.g., WOOD & NASSAU, 1968). The OH-stretching IR spectra of beryl have been extensively studied (see KOLESOV & GEIGER, 2000 and references therein). However there is no general consensus on the assignment of the observed bands to structural configurations. Much confusion probably arises from the fact that most beryls contain simultaneously both types of water, and there is no knowledge on the effect of a possible interaction between them. We present here a single-crystal, polarized-light FTIR study (done on a NicPlan microscope, equipped with a MCT detector and a gold-wire polarizer) on oriented polished sections of a flux-grown emerald. Contrary to the synthesis conditions, the emerald was found to contain low amounts of type II water exclusively, possibly associated with trace alkali ions in the channels (detected by EMPA). On the (100) section, the **E**⊥c spectrum shows a unique sharp and intense band at 3643 cm^{-1}, while the **E**//c spectrum consists of two low-intensity bands at 3643 and 3587 cm^{-1}, respectively. Based on this pleochroic behavior, the 3643 cm^{-1} band is assigned to the ν_3 antisymmetric stretching of type II water. The second, minor band at 3587 cm^{-1} has maximum absorbance for **E**//*c*; it is assigned to the ν_1 symmetric stretching of type II water, as also suggested by the intensity ratio I_{3643} I_{3587} close to 1:20. The polarization of the observed bands definitely indicates that type II water has its molecular axis //*c* with its H...H vector ⊥*c*. The integrated molar absorbance for beryl, never calibrated so far, has been determined from the curve of LIBOWITZKY & ROSSMAN (1997) to be ε_I at 3643 cm^{-1} = 27126 l mol^{-1} cm^{-2} This value allows to calculate a water content of 30 ppm for our synthetic, nominally anhydrous, beryl.

References

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