Lithiums role in the crystal chemistry of beryl

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We have investigated the Li, Be, Al and Si contents of both synthetic and natural beryl crystals including samples obtained from a spectrum of lithologies representing both metamorphic-metasomatic as well as pegmatitic sources. The absolute contents of the various elements were investigated by electron microprobe and SIMS, in addition to X-ray powder diffraction and FTIR-spectroscopy to characterize the structural details. This work focuses on the distribution of Be²⁺, Al³⁺ and Si⁴⁺ on the tetrahedral sites, and on the substitution mechanism responsible for the incorporation of Li⁺ into the beryl structure. Both BeO and Li₂O were successfully quantified by SIMS at the circa 5 μ m scale. For the 12 crystals, which have been studied so far, the BeO concentrations range between 12 to 14 wt%, whereas Li concentrations are in the range of ca 40 $\mu g/g$ to 1150 $\mu g/g$. The accompanying range of SiO₂-contents is $\approx 62 \text{ to } 67$ wt%, and that of Al₂O₃ 14.4 to 18.5 wt%. Detailed analysis of polarized IR spectra in the regions of H₂O vibrations, measured on beryl crystals with different Li content, was carried out to check for the possible involvement of OH with the Li substitution. Results and possible interpretation of two crystals with high (4645 $\mu g/g$ wet chemistry determination) and low Li content (55 $\mu g/g$ SIMS determination; 90 $\mu g/g$ wet chemistry determination) resp., show significantly larger lattice constants of the Li-rich beryl: a = 9.2161(3) Å, c = 9.2001(6) Å and V = 676.74(6) Å³ 2 σ compared to a = 9.2061(4) Å, c = 9.1873(5) Å, V = 674.34(5) Å³.

Our data show no clear correlation between Be and Li in the studied samples. Li is heterogeneously distributed in most crystals, especially in hydrothermal grown synthetic samples. These results contradict the conclusion about Li-Be substitution as a predominant mechanism of Li incorporation into the beryl structure (e.g. for Cs-Li beryl: Hawthorne and Cerny, 1977). Other schemes of heterovalent substitutions involving Li should play an important role in both natural and synthetic beryl.

References

Hawthorne FC, and Cerny P (1977) The alkali-metal positions in Cs-Li beryl. Can Mineral 15: 414-421

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