Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.10025

Predicting the Crystal Structure of Beryl from Chemical Analyses

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Crystal structure prediction is a challenging topic. A model has not previously been developed that uses the chemical composition of a known mineral to determine the complete crystal structure, including all major bond lengths and angles, atomic coordinates, polyhedral volumes and distortions, and unit cell parameters. The mineral beryl is used here to create such a model.

Beryl ($Be_3Al_2Si_6O_{18}$) is an ideal mineral to prove that modeling the crystal structure using chemistry is possible: the base structure is known, it has two cation sites that experience substitutions, and these do not occur simultaneously. This research uses single-crystal X-ray diffraction and electron-probe micro-analyses on 80 samples to create the model. The model's validity is tested with 33 samples to verify that the measured structures fall within the predicted boundaries.

Results indicate that a complete crystal structure of beryl can be calculated accurately using chemical composition by utilizing the average ionic radii of the measured cations within the Al- and Be-sites. Beryl can be separated into two categories: octahedrally and tetrahedrally trending. The full structure is predictable using the Al-site average ionic radii for octahedrally trending beryl, or the Be-site average ionic radius for tetrahedrally trending beryl. Red beryl (differentiated by high Fe and Mn) has a slightly different trend, forming a subset of octahedrally trending beryl. This model makes it possible to explore the limitations on the beryl structure and the possibility of unusual cation substitutions. It is robust for all true beryl up to a high limit of substitutions, but not for other beryl group minerals.

This research is beneficial for beryl studies, which will be able to determine crystal structures during standard chemical analyses. It enables the creation of an extensive beryl database, aids comparisons of natural beryl to synthetics, and helps provide further guidance on provenance studies. It also invites future crystal structure prediction research. This approach is applicable to broader fields, as crystal structures are linked to the physical characteristics of minerals and rocks in which they form.