

## Molecular water in beryl, ${}^{\text{VI}}\text{Al}_2 [\text{Be}_3\text{Si}_6\text{O}_{18}] \cdot n\text{H}_2\text{O}$ , as a function of pressure and temperature: An experimental study

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### ABSTRACT

The incorporation of molecular water into the *c*-parallel structural channels in end-member beryl  ${}^{\text{VI}}\text{Al}_2 [\text{Be}_3\text{Si}_6\text{O}_{18}] \cdot n\text{H}_2\text{O}$ , where  $n_{\text{H}_2\text{O}} = 1.00$  corresponds to 3.24 wt%  $\text{H}_2\text{O}$ , was studied experimentally in the temperature-pressure range 400–950 °C and 1–14.5 kbar ( $P_{\text{H}_2\text{O}} = P_{\text{tot}}$ ). Time-dependent studies ensured that the incorporation of water by beryl had reached the equilibrium  $n_{\text{H}_2\text{O}}$  values in the hydration experiments.

Increasing water contents were found to enhance the refractive indices of beryl as follows:

$$n_e = 1.5585 + 0.0080 \cdot \text{wt\% H}_2\text{O} \quad (r = 0.986)$$

$$n_w = 1.5616 + 0.0086 \cdot \text{wt\% H}_2\text{O} \quad (r = 0.978)$$

These relations were used to determine the water contents attained in the equilibrium experiments, and were calibrated using synthetic beryls, the water contents of which had been determined gravimetrically with an accuracy of  $\pm 0.06$  wt%  $\text{H}_2\text{O}$ . The incorporation of water into the structural channels of beryl leaves the hexagonal *a*-axis unchanged,  $a = 9.2110(10)$  Å, *c* and *V* increase as:

$$c \text{ (Å)} = 9.1893 + 0.0020 \cdot \text{wt\% H}_2\text{O} \quad (r = 0.974)$$

$$V \text{ (Å}^3\text{)} = 674.98 + 0.203 \cdot \text{wt\% H}_2\text{O} \quad (r = 0.936)$$

Two isobars at 3.4 and 10.8 kbar with  $P_{\text{H}_2\text{O}} = P_{\text{total}}$  could be modeled as:

$$\text{wt\% H}_2\text{O} (P) = a - bT \text{ (}^\circ\text{C)} + cT^2 \text{ (}^\circ\text{C)}^2$$

$$3.4 \text{ kbar: } a = 4.10, b = 5.90 \cdot 10^{-3}, c = 0.31 \cdot 10^{-5} \quad (r = 0.963)$$

$$10.8 \text{ kbar: } a = 3.31, b = 0.514 \cdot 10^{-3}, c = 0.00 \quad (r = 0.941)$$

Similarly, the two isotherms at 600 and 900 °C could be modeled as:

$$\text{wt\% H}_2\text{O} (T) = a + bP \text{ (kbar)} - cP^2 \text{ (kbar)}^2$$

$$500 \text{ }^\circ\text{C: } a = 0.94, b = 0.261, c = 0.0075 \quad (r = 0.949)$$

$$900 \text{ }^\circ\text{C: } a = 0.19, b = 0.331, c = 0.0092 \quad (r = 0.964)$$

These relations together with data points from additional experiments were used to construct a ( $P_{\text{H}_2\text{O}} = P_{\text{tot}}$ ) – *T* field of isohydrans for the system end-member beryl– $\text{H}_2\text{O}$ . Comparing  $n_{\text{H}_2\text{O}}$ –*P* sections at 600 °C for beryl obtained in this study with data for Mg-cordierite obtained from the literature, proves nearly the same equilibrium contents of water in both minerals.