A refined zirconium-in-rutile thermometer

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Abstract

The zirconium-in-rutile thermometer enjoys widespread use, but confidence in its accuracy is limited because experiments were conducted at higher temperatures than many rutile-bearing rocks and calibration uncertainties have not been quantitatively assessed. Refined calibrations were developed using bootstrap regression to minimize residuals in the natural logarithm of the equilibrium constant, based on experiments only ($n = 32$) and on a combined compilation of experiments and natural data ($n = 94$, total). Rearranging the regression to solve for T, and expressing Zr concentration (C) in parts per million (μg/g), the calibrations in the α-quartz stability field are:

Experimental data set:

$$T(°C) = \frac{68740 + 0.441 \cdot P(\text{bars}) - 0.114 \cdot C(\text{ppm})}{129.76 - R \cdot \ln\left[C(\text{ppm})\right]} - 273.15.$$

Combined data set:

$$T(°C) = \frac{71360 + 0.378 \cdot P(\text{bars}) - 0.130 \cdot C(\text{ppm})}{130.66 - R \cdot \ln\left[C(\text{ppm})\right]} - 273.1.$$

Thermodynamics of the quartz-coesite transition as applied to the calibration for α-quartz yields calibrations for the coesite stability field:

Experimental data set

$$T(°C) = \frac{71290 + 0.310 \cdot P(\text{bars}) - 0.114 \cdot C(\text{ppm})}{128.76 - R \cdot \ln\left[C(\text{ppm})\right]} - 273.15.$$

Combined data set:

$$T(°C) = \frac{73910 + 0.247 \cdot P(\text{bars}) - 0.130 \cdot C(\text{ppm})}{129.65 - R \cdot \ln\left[C(\text{ppm})\right]} - 273.15.$$

Propagated temperature uncertainties are ±20–30 °C (2σ) for the experimental data set calibration, and ±10–15 °C (2σ) for the combined data set. Compared to previous experimental calibrations, the refined thermometer predicts temperatures up to 40 °C lower for $T \leq 550$ °C, and systematically higher temperatures for $T > 800$ °C. With careful attention to distributions of Zr in rutile grains, precisions of ±5 °C and accuracies ~±15 °C may be possible, although a poor understanding of how to select compositions for thermometry will typically lead to larger uncertainties. The ZiR calibration promises continued high-precision and accurate thermometry, and possibly improved thermodynamic properties, but the sources of compositional variability in rutile warrant further scrutiny.

Keywords: Zirconium, rutile, thermometry, bootstrap regression, errors