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Igneous thermometers and barometers based on plagioclase + liquid equilibria: Tests of some existing models and new calibrations

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ABSTRACT

Although many formulations of plagioclase + liquid equilibria have been calibrated in the last decade, few models specifically address the issue of temperature (T) prediction. Moreover, for those that do, T error is not addressed, greatly limiting their use as geothermometers. Several recent models of plagioclase-liquid equilibria are thus tested for their ability to recover T from their calibration data, and predict T from experiments not used for calibration. The models of Sugawara (2001) and Ghiorso et al. (1995, 2002) outperform earlier calibrations. These models perform reasonably well at $T > 1100$ °C, though recovery and prediction of T is less precise for hydrous compositions. In addition, these models cannot be integrated with geo-hygrometers, or other mineral-melt thermometers and barometers; the following expression predicts T with up to 40% greater precision:

$$\frac{10^4}{T(\mathrm{K})} = 6.12 + 0.257\ln\left(\frac{[\mathrm{An}^{\mathrm{pl}}]}{\left[\mathrm{Ca}^{\mathrm{liq}}\left(\mathrm{Al}^{\mathrm{liq}}\right)^2\left(\mathrm{Si}^{\mathrm{liq}}\right)^2\right]}\right) - 3.166[\mathrm{Ca}^{\mathrm{liq}}] + 0.2166[\mathrm{H_2O}^{\mathrm{liq}}] - 3.137\left[\frac{\mathrm{Al}^{\mathrm{liq}}}{\mathrm{Al}^{\mathrm{liq}} + \mathrm{Si}^{\mathrm{liq}}}\right] + 1.216[\mathrm{Ab}^{\mathrm{pl}}]^2 - 2.475\times10^{-2}[P(\mathrm{kbar})] \quad (1)$$

Because these thermometers are pressure (P) sensitive, a temperature-sensitive barometer was also developed:

$$P(\mathrm{kbar}) = -42.2 + 4.94\times10^{-2}[T(\mathrm{K})] + 1.16\times10^{-2}T(\mathrm{K})\ln\left(\frac{[\mathrm{Ab}^{\mathrm{pl}}\mathrm{Al}^{\mathrm{liq}}\mathrm{Ca}^{\mathrm{liq}}]}{[\mathrm{An}^{\mathrm{pl}}\mathrm{Na}^{\mathrm{liq}}\mathrm{Si}^{\mathrm{liq}}]}\right) - 382.3[\mathrm{Si}^{\mathrm{liq}}]^2 + 514.2[\mathrm{Si}^{\mathrm{liq}}]^3 - 19.6\ln[\mathrm{Ab}^{\mathrm{pl}}] - 139.8[\mathrm{Ca}^{\mathrm{liq}}] + 287.2[\mathrm{Na}^{\mathrm{liq}}] + 163.9[\mathrm{K}^{\mathrm{liq}}] \quad (2)$$

In these models, T is in Kelvins and P is in kbar. $\mathrm{An}^{\mathrm{pl}}$ and $\mathrm{Ab}^{\mathrm{pl}}$ are the fractions of anorthite and albite in plagioclase, calculated as cation fractions: An = $\mathrm{CaO/(CaO + NaO_{0.5} + KO_{0.5})}$ and Ab = $\mathrm{NaO_{0.5}/(CaO+NaO_{0.5}+KO_{0.5})}$. Terms such as $\mathrm{Al}^{\mathrm{liq}}$ refer to the anhydrous cation fraction of Al in the liquid; H_2O in Equation 1 is in units of wt%. Errors on these models are comparable to those for clinopyroxene thermobarometers: In Equation 1, $R = 0.99$ and the standard error of estimate (SEE) is 23 K; for Equation 2, $R = 0.94$ and the SEE is 1.8 kbar. The models successfully recover mean pressures for experimental data that are not used for calibration, and are furthermore able to recover near-1-atm P estimates for volcanic rocks from Kilauea, Hawaii, which are thought to have crystallized at or very near Earth's surface.