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Titanium in muscovite, biotite, and hornblende: Modeling, thermometry, and rutile activities of metapelites and amphibolites

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ABSTRACT

Reactions involving the $^{VI}Ti^{IV}Al$-$^{VI}Al^{IV}Si$ exchange in muscovite, biotite, and hornblende were calibrated thermodynamically using a set of experimental and natural data in rutile- plus quartz/coesite-bearing assemblages. The specific respective reactions are

$$K(Al_2)(AlSi_3)O_{10}(OH)_2 + TiO_2 = K(AlTi)(Al_2Si_2)O_{10}(OH)_2 + SiO_2 \quad (R1)$$

$$K(\square MgAl)Si_4O_{10}(OH)_2 + TiO_2 = K(\square MgTi)AlSi_3O_{10}(OH)_2 + SiO_2 \quad (R2)$$

$$Ca_2Mg_3Al_2Al_2Si_6O_{22}(OH)_2 + 2TiO_2 = Ca_2Mg_3Ti_2Al_4Si_4O_{22}(OH)_2 + 2SiO_2. \quad (R3)$$

Ideal mixing on octahedral or octahedral plus tetrahedral sites and a non-ideal van Laar solution model yield the best regression results for thermodynamic fit parameters, with R^2 values of 0.98–1.00. Isopleths of the equilibrium constant (K_{eq}) show minimal pressure dependencies of <1 °C/kbar, implying that the equilibria are poor barometers. Model reproducibility of the ideal portion of the equilibrium constant (K_{id}) is excellent (ca. ±0.1 to 0.3, 2σ), but the absolute value of the combined term $\Delta S+K_{id}$ is quite small (absolute values from 0 to 4), so calibration residuals propagate to temperature errors >±50–100 °C, 1σ. Whereas the consistency of a mica or hornblende composition with a known *T* can be evaluated precisely, Ti chemistry in these reactions is sensitive to composition and does not resolve *T* (or *P*) well. The activity of TiO_2 in rutile [*a*(rt)] was also evaluated using both the garnet-rutile-ilmenite-plagioclase-quartz (GRIPS) equilibrium and our new calibrations in rutile-absent, ilmenite-bearing rocks whose peak *P-T* conditions are otherwise known. Metapelites have average *a*(rt) of 0.9 (GRIPS) and 0.8 (R1), whereas amphibolites have *a*(rt) of 0.95 (GRIPS and R3). A value for *a*(rt) of 0.80 ± 0.20 (metapelites) and 0.95 +0.05/–0.25 (amphibolites) is recommended for trace-element thermomobarometers in ilmenite-bearing, rutile-absent rocks. The dependence of Ti contents of minerals on *a*(rt) and the reequilibration of Ti during metamorphic reactions both deserve further exploration, and may affect application of trace-element thermobarometers.

Keywords: Titanium, rutile, muscovite, biotite, hornblende