Appendix B: How to use the plagioclase-liquid hygrometer/thermometer

The plagioclase-liquid hygrometer/thermometer model is available as a Visual Basic program that runs on Excel 2004. It can be downloaded from the Data Repository. For readers who would like to create their own spreadsheet of this plagioclase-liquid program, a brief outline of how to perform the calculation is provided below.

Calculation of wt% H_2O

Step 1. Begin with the model regression equation (Eq. 25), which has four terms:

$$wt\%H_2O = m'x + a'' + \frac{b''}{T} + \sum d_i''X_i \qquad (25)$$

Step 2. The first term requires calculation of *x*, which is defined by Equation 22:

$$x = \left[\frac{\Delta H^o(T)}{RT} - \frac{\Delta S^o(T)}{R} + \frac{\int_1^P \Delta V_T^o(P)dP}{RT} + \ln K^*\right]. \qquad (22)$$

Step 2a. To calculate $\Delta H°$(T) for the reaction, use Equation 3b:

$$\Delta H°(\mathrm{T}) = \Delta H^{An}{}_{fusion}(\mathrm{T}) - \Delta H^{Ab}{}_{fusion}(\mathrm{T}) \qquad (3b)$$

and Equation 8 for An (anorthite) and Ab (albite), respectively, using the data in Table 1:

$$\Delta H_{fus}(T_m) + \Delta H_{fus}(T_m) + \int_{\mathrm{T}m}^{\mathrm{T}}[\mathrm{C}^{liq}{}_p(T) - \mathrm{C}^{xtl}{}_p(T)]dT. \qquad (8)$$

Step 2b. To calculate $\Delta S°$(T) for the reaction, use Equation 4:

$$\Delta S°(T) = \Delta S_{fus}{}^{An}(T) - \Delta S_{fus}{}^{Ab}(T) \qquad (4)$$

and Equation 9 for An (anorthite) and Ab (albite), respectively, using the data in Table 1:

$$\Delta S_{fus}(T) = \Delta S_{fus}(T_m) + \int_{T_m}^{T}\left(\frac{C_p^{liq}(T) - C_p^{xtl}(T)}{T}\right)dT. \qquad (9)$$

Step 2c. To calculate $\int_{1bar}^{P}\Delta V_T^o(P)dP$, use Equation 13 and the data in Table 1:

$$\int_{1bar}^{P}\Delta V_T^o(P)dP = \left[V_{T,1bar}^{liquid\ An} - V_{T,1bar}^{crystal\ An} - V_{T,1bar}^{liquid\ Ab} + V_{T,1bar}^{crystal\ Ab}\right](P-1)$$
$$+\frac{1}{2}\left[\left(\frac{\partial V}{\partial P}\right)_T^{liq\ An} - \left(\frac{\partial V}{\partial P}\right)_T^{crystal\ An} - \left(\frac{\partial V}{\partial P}\right)_T^{liq\ Ab} + \left(\frac{\partial V}{\partial P}\right)_T^{crystal\ Ab}\right](P^2-1). \qquad (13)$$

Step 2d. To calculate ln$K$*, use Equation 19:

$$\ln K^* = \ln\left(\frac{X^{ideal\ \ liquid}_{CaAl_2Si_2O_8}}{X^{ideal\ \ liquid}_{NaAlSi_3O_8}}\right) + \ln\left(\frac{a^{crystal}_{NaAlSi_3O_8}}{a^{crystal}_{CaAl_2Si_2O_8}}\right). \qquad (19)$$

Calculate the first term in Equation 19 with Equations 16a and 16b:

$$X^{ideal\ \ liquid}_{CaAl_2Si_2O_8} = 64.0\left(X^{liq}_{CaO}\right)\left(X^{liq}_{Al_2O_3}\right)\left(X^{liq}_{SiO_2}\right)^2 \qquad (16a)$$

$$X^{ideal\ \ liquid}_{NaAlSi_3O_8} = 18.963\left(X^{liq}_{Na_2O}\right)^{0.5}\left(X^{liq}_{Al_2O_3}\right)^{0.5}\left(X^{liq}_{SiO_2}\right)^3. \qquad (16b)$$

Calculate the second term in Equation 19, use the THERMOCALC program of Holland et al. (1998). It can be downloaded (http://www.earthsci.unimelb.edu.au/tpg/thermocalc/). In this program, input the wt% oxide composition of plagioclase; the output is the activity of the two components, $a^{crystal}_{NaAlSi3O8}$ and $a^{crystal}_{CaAl2Si2O8}$.

Step 2e. Add the four terms calculated in Steps 2a–2d, and then multiply their sum by the fitted coefficient *m′* (=1.91) in Table 2. This is the first term in Equation 25.

Step 3. Take the value in Step 2e and add the coefficient *a″* (= 13.53) in Table 2.

Step 4. Take the value in Step 3 and add coefficient *b″* (=2.95) (Table 2) divided by temperature (in degrees Kelvin).

Step 5. Convert the anhydrous liquid composition from wt% oxide (SiO_2, TiO_2, Al_2O_3, FeO^T, MgO, CaO, Na_2O, and K_2O) into mole fractions. Then calculate the final term in Equation 25 with the fitted terms from Table 2:

$$\Sigma d_i''X_i = -9.82X_{SiO2} + 24.49X_{Al2O3} - 5.87X_{FeOT} - 15.56X_{MgO} + 17.10X_{CaO}$$

Add this value to the value calculated in Step 4. This is the calculated value for wt% H_2O.

Calculation of Temperature:

To calculate temperature using this model, simply adjust the input temperature [in calculations in Steps 2a, 2b, 2c, and 2d (THERMOCALC part) and Step 4] until the calculated wt% H_2O value matches the known value.