

## 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<sub>2</sub>O

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

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

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

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

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

$$\Delta H^o(T) = \Delta H_{fusion}^{An}(T) - \Delta H_{fusion}^{Ab}(T) \quad (3b)$$

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

$$\Delta H_{fus}(T_m) + \Delta H_{fus}(T_m) + \int_{T_m}^T [C_p^{liq}(T) - C_p^{xtl}(T)] dT. \quad (8)$$

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

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

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

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

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

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

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

$$\ln K^* = \ln \left( \frac{X_{CaAl_2Si_2O_8}^{ideal \ liquid}}{X_{NaAlSi_3O_8}^{ideal \ liquid}} \right) + \ln \left( \frac{a_{NaAlSi_3O_8}^{crystal}}{a_{CaAl_2Si_2O_8}^{crystal}} \right) \quad (19)$$

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

$$X_{CaAl_2Si_2O_8}^{ideal \ liquid} = 64.0 (X_{CaO}^{liq}) (X_{Al_2O_3}^{liq}) (X_{SiO_2}^{liq})^2 \quad (16a)$$

$$X_{NaAlSi_3O_8}^{ideal \ liquid} = 18.963 (X_{Na_2O}^{liq})^{0.5} (X_{Al_2O_3}^{liq})^{0.5} (X_{SiO_2}^{liq})^3 \quad (16b)$$

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,  $a_{NaAlSi_3O_8}^{crystal}$  and  $a_{CaAl_2Si_2O_8}^{crystal}$ .

**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:

$$\sum d_i'' X_i = -9.82 X_{SiO_2} + 24.49 X_{Al_2O_3} - 5.87 X_{FeO^T} - 15.56 X_{MgO} + 17.10 X_{CaO}$$

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.