ALBITE, JADEITE AND QUARTZ PHASE DIAGRAM

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Reference: Daniel V. Schroeder, *An Introduction to Thermal Physics*, (Addison-Wesley, 2000) - Problem 5.40.

Here's an example of applying the Gibbs energy and the Clausius-Clapeyron relation to a case where one solid (albite, with formula $NaAlSi_3O_8$) dissociates into two other solids (jadeite, with formula $NaAlSi_2O_6$, and quartz, SiO_2) under the reversible reaction

$$NaAlSi_3O_8 \longleftrightarrow NaAlSi_2O_6 + SiO_2 \qquad (1)$$
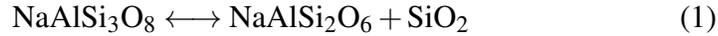
To get a rough phase diagram, we need to first find one point on the phase boundary by using the Gibbs free energy, as we did for aluminum silicate, and then find the slope of the phase boundary using the Clausius-Clapeyron relation.

First, we use

$$\left(\frac{\partial G}{\partial P}\right)_{T,N} = V \qquad (2)$$

Ignoring compressibility, we can assume that V is constant as the pressure is increased. The molar volumes, in m^3, for the three forms are, from the data in Schroeder's book: $V_a = 100.07 \times 10^{-6}$, $V_j = 60.4 \times 10^{-6}$ and $V_q = 22.69 \times 10^{-6}$. Since the pressures involved are in the kilobar region, we can take the Gibbs data (given for $P = 1$ bar) to be the values for $P \approx 0$ and we get, with energy in kJ and pressure in kbar (with 1 kbar $= 10^8$ Pa):

$$
\begin{align}
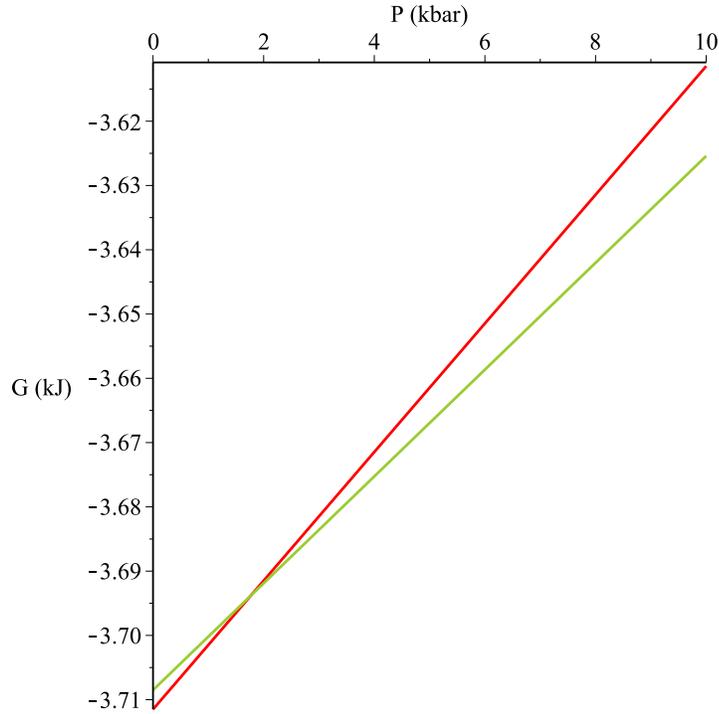G_a &= -3711.5 + 10.007P & (3)\\
G_j &= -2852.1 + 6.04P & (4)\\
G_q &= -856.4 + 2.269P & (5)
\end{align}
$$

For the reaction 1, the relevant Gibbs energy for the RHS is the sum $G_j + G_q$, so the energies we want to compare to find the stable form are

$$
\begin{align}
G_a &= -3711.5 + 10.007P & (6)\\
G_{jq} &= -3708.5 + 8.309P & (7)
\end{align}
$$

Plotting these two lines we get

The red line is albite and the green line is jadeite + quartz. At low pressure, albite has the lower Gibbs energy so is the stable form. The lines cross at a pressure of $P_{ajq} = 1.77$ kbar so at that pressure and a temperature of 298 K, the two sides are in equilibrium. For higher pressures, the stable form is jadeite + quartz.

We could use this point as one point on the phase diagram, but we can also use the earlier method that we applied to aluminum silicate. The difference in Gibbs energy between the two sides of the equation is

$$\Delta G\left(T_2\right) = \Delta G\left(T_1\right) - \Delta S\left(T_2 - T_1\right) \tag{8}$$

The entropies are, in units of kJ K^{-1}: $S_a = 0.2074$, $S_j = 0.1335$ and $S_q = 0.04184$ so, taking $T_1 = 298$ K and $\Delta G\left(298\right) = G_a - G_{jq}$ evaluated at $P = 0$ from 6, we have

$$\Delta G\left(T_2\right) = -3.0 - 0.03206\left(T - 298\right) \tag{9}$$

The phase boundary passes through the point where $\Delta G = 0$, which occurs at $T = 204.4$ K. From the Clausius-Clapeyron equation, the slope of the boundary at this point is
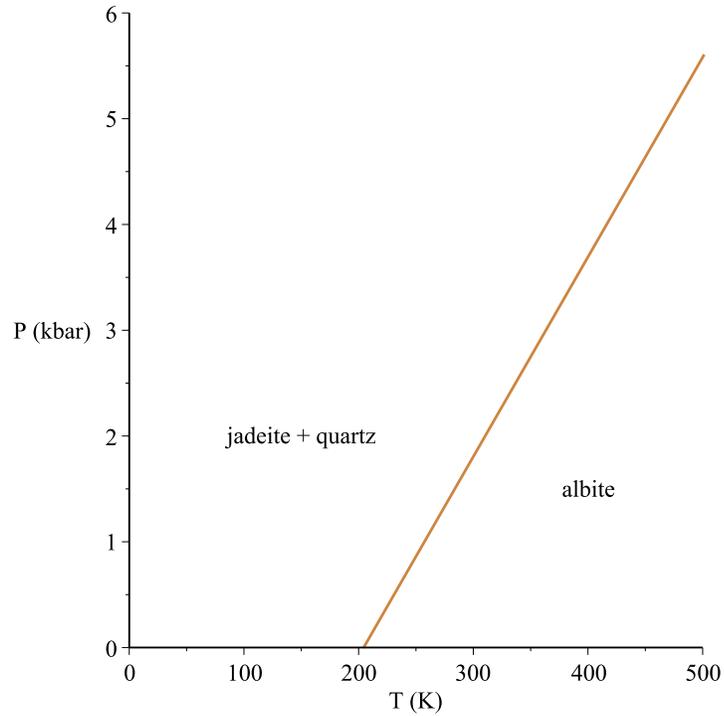
$$\frac{dP}{dT} = \frac{S_a - \left(S_j + S_q\right)}{V_a - \left(V_j + V_q\right)} = 0.0189 \text{ kbar K}^{-1} \tag{10}$$

Thus the phase boundary has the equation

$$P = \frac{dP}{dT}(T - 204.4) \tag{11}$$
$$= 0.0189\,(T - 204.4) \tag{12}$$

A plot of the boundary looks like this:

As always, this is only a crude approximation as it disregards variations in entropy and volume as the pressure and temperature are changed, and extrapolates the entire boundary from the slope at a single point.