

ALUMINUM SILICATE PHASE DIAGRAM

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Reference: Daniel V. Schroeder, *An Introduction to Thermal Physics*, (Addison-Wesley, 2000) - Problem 5.39.

We can use the Clausius-Clapeyron relation to plot an estimate of the phase diagram of the three forms of aluminum silicate (kyanite, andalusite and sillimanite). From the entropy and volume data in Schroeder's book, we can calculate the slope of the phase boundary:

$$\left. \frac{dP}{dT} \right|_{12} = \frac{S_1 - S_2}{V_1 - V_2} \quad (1)$$

where the subscripts refer to two different phases. Since we are given data for only one temperature ($T = 298 \text{ K}$) and one pressure ($P = 1 \text{ bar}$), we'll need to assume that the slopes are constant over a wider range of temperatures and pressures to get a phase diagram. With this proviso, we have

$$\left. \frac{dP}{dT} \right|_{ks} = \frac{S_k - S_s}{V_k - V_s} \quad (2)$$

$$= \frac{83.81 - 96.11}{(44.09 - 49.9) \times 10^{-6}} \quad (3)$$

$$= 2.12 \times 10^6 \text{ Pa K}^{-1} \quad (4)$$

$$\left. \frac{dP}{dT} \right|_{as} = \frac{93.22 - 96.11}{(51.53 - 49.9) \times 10^{-6}} \quad (5)$$

$$= -1.77 \times 10^6 \text{ Pa K}^{-1} \quad (6)$$

$$\left. \frac{dP}{dT} \right|_{ka} = \frac{83.81 - 93.22}{(44.09 - 51.53) \times 10^{-6}} \quad (7)$$

$$= 1.26 \times 10^6 \text{ Pa K}^{-1} \quad (8)$$

From our earlier calculations, we estimated the temperature T_{12} of each phase transition at a pressure of $P = 1 \text{ bar}$. We can write the phase boundary as

$$P(T) = P(T_{12}) + \left. \frac{dP}{dT} \right|_{12} (T - T_{12}) \quad (9)$$

A given transition occurs when $\Delta G_{12} = 0$, that is, the Gibbs free energy difference between the two phases is zero. For the phase transitions we have

$$\Delta G_{ks} = -2.89 + 12.30 \times 10^{-3} (T_{ks} - 298) = 0 \quad (10)$$

$$T_{ks} = 533 \text{ K} \quad (11)$$

$$\Delta G_{ka} = -1.22 + 9.41 \times 10^{-3} (T_{ka} - 298) = 0 \quad (12)$$

$$T_{ka} = 428 \text{ K} \quad (13)$$

$$\Delta G_{as} = -1.67 + 2.89 \times 10^{-3} (T_{as} - 298) = 0 \quad (14)$$

$$T_{as} = 876 \text{ K} \quad (15)$$

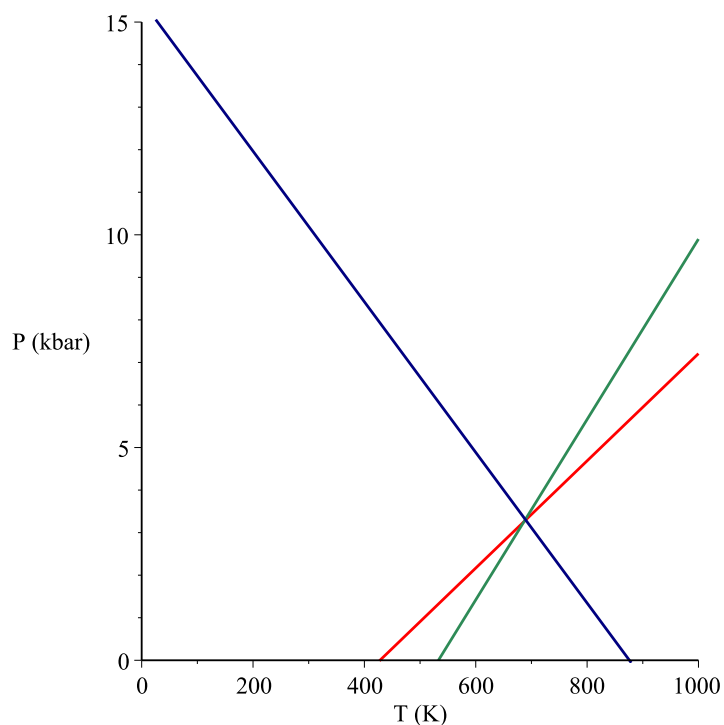
Since the pressure of 1 bar is effectively zero (as we're dealing with pressures of kilobars in the graph), we can convert pressure to kilobars in 9 by dividing by 10^8 and get

$$P_{ks} = 0.0212 (T - 533) \quad (16)$$

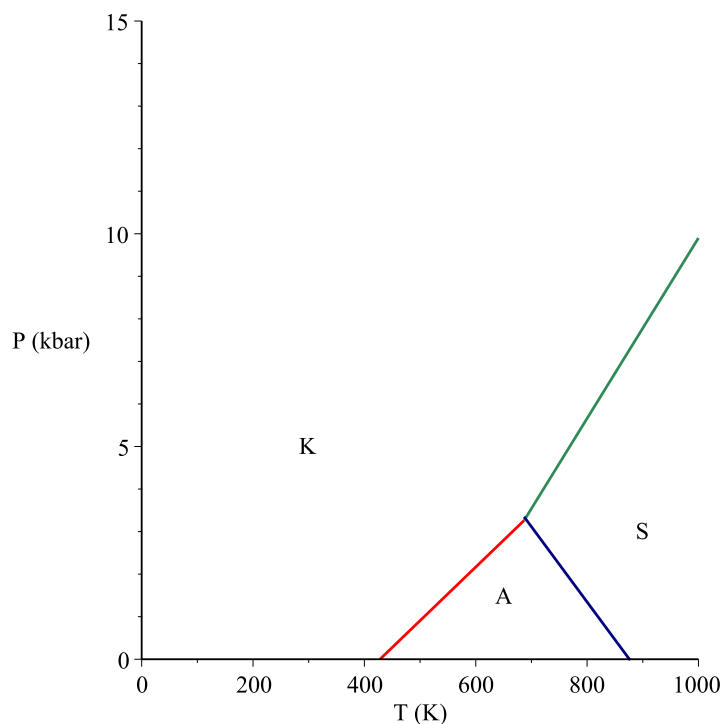
$$P_{ka} = 0.0126 (T - 428) \quad (17)$$

$$P_{as} = -0.0177 (T - 876) \quad (18)$$

Plotting these lines gives us:



The red line is the kyanite-andalusite boundary, green is kyanite-sillimanite and blue is andalusite-sillimanite. However, from our earlier calculation with the Gibbs free energy, we know that for $P = 1$ bar, kyanite is the stable form for $T < 428$ K, then andalusite for $428 \text{ K} < T < 876$ K and finally sillimanite for $T > 876$ K. Thus the portion of the green line below the intersection point is not part of the phase boundary, nor are the portions of the red and blue lines above the intersection point. Removing these gives the final phase diagram:



The region where each of the three forms is stable is labelled with (K)yanite, (A)ndalusite and (S)illimanite.

The triple point is the point where all three phases are in equilibrium and can be found from the intersection point between any two of the lines above. The temperature is found by equating 16 and 17 and gives

$$T_3 = 687 \text{ K} \quad (19)$$

The corresponding pressure is

$$P_3 = 3.26 \text{ kbar} \quad (20)$$

As with the earlier calculations involving the Gibbs energies, this diagram is probably not very accurate, since the entropy difference between any two phases is probably not exactly constant.