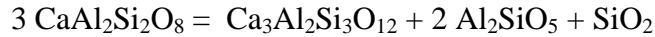


PROBLEM SET #7

All of the questions pertain to the following reaction:



Thermodynamic data:

Anorthite:  $H_f^\circ = -4229.10 \text{ kJ/mole}$   
 $S(1 \text{ bar}, 298\text{K}) = 199.3 \text{ J/mole-K}$   
 $V(1 \text{ bar}, 298\text{K}) = 100.79 \text{ cm}^3/\text{mole}$   
 $C_p = 5.1683 \times 10^2 - 9.2492 \times 10^{-2}(T) + 4.1883 \times 10^{-5}(T)^2 - 4.5885 \times 10^{-3}T^{-0.5} - 1.4085 \times 10^{-6}T^{-2}$   
(valid between 298K and 1800K)

Grossular:  $H_f^\circ = -6643.14 \text{ kJ/mole}$   
 $S(1 \text{ bar}, 298\text{K}) = 255.5 \text{ J/mole-K}$   
 $V(1 \text{ bar}, 298\text{K}) = 125.3 \text{ cm}^3/\text{mole}$   
 $C_p = 1.5293 \times 10^3 - 0.699(T) + 2.53 \times 10^{-4}(T)^2 - 1.8943 \times 10^{-4}T^{0.5} + 7.4426 \times 10^{-6}T^{-2}$   
(valid between 298K and 1200K)

Kyanite:  $H_f^\circ = -2591.73 \text{ kJ/mole}$   
 $S(1 \text{ bar}, 298\text{K}) = 83.76 \text{ J/mole-K}$   
 $V(1 \text{ bar}, 298\text{K}) = 44.090 \text{ cm}^3/\text{mole}$   
 $C_p = 4.3612 \times 10^2 - 0.13576(T) + 4.7236 \times 10^{-5}(T)^2 - 4.8027 \times 10^{-3}T^{-0.5}$   
(valid between 298K and 1500K)

Quartz:  $H_f^\circ = -910.70 \text{ kJ/mole}$   
 $S(1 \text{ bar}, 298\text{K}) = 41.46 \text{ J/mole-K}$   
 $V(1 \text{ bar}, 298\text{K}) = 22.688 \text{ cm}^3/\text{mole}$   
 $C_p = 44.603 + 3.7754 \times 10^{-2}(T) - 1.0018 \times 10^{-6}T^{-2}$   
(valid between 298K and 844K)

1. What is the change in volume for this reaction ( $\Delta V_R(1 \text{ bar}, 298\text{K})$ ) at 298K and 1 bar? Are the products or reactants denser?
2. What is the change in enthalpy for this reaction ( $\Delta H_R(1 \text{ bar}, 298\text{K})$ ) at 298K and 1 bar? Is the reaction exothermic or endothermic?
3. What is the change in internal energy for this reaction ( $\Delta E_R(1 \text{ bar}, 298\text{K})$ ) at 298K and 1 bar? For this reaction, under these conditions is q or w the larger term?
4. What is the change in entropy for this reaction ( $\Delta S_R(1 \text{ bar}, 298\text{K})$ ) at 298K and 1 bar? Are the products or reactants more disordered?

5. What is the change in Gibbs Free Energy for this reaction ( $\Delta G_R(1\text{bar}, 298\text{K})$ ) at 298K and 1 bar? Are the products or reactants stable under these conditions?
6. Assuming  $\Delta S_R$  and  $\Delta V_R$  are constant with P and T, at 1 bar and what temperature is  $\Delta G_R = 0$ ? What is the change in enthalpy for the reaction at this T and 1 bar?
7. Assuming  $\Delta S_R$  and  $\Delta V_R$  are constant with P, at what pressure is  $\Delta G_R = 0$  when T = 700 K?
8. What is the Clapeyron slope of the reaction?
9. Using your answers to problems 6 & 7 and assuming that  $\Delta S$  and  $\Delta V$  are constant with T and P, plot the P-T phase diagram and label the fields. In your phase diagram, please note where  $\Delta G_R > 0$ ,  $\Delta G_R < 0$ , and  $\Delta G_R = 0$ .
10. Al in Grossular and Kyanite has the same coordination number. The coordination number for Al in Grossular is different from that in Anorthite. Which (Grossular or Anorthite) would you guess has a higher coordination number for Al? Why?