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89.304 - IGNEOUS & METAMORPHIC PETROLOGY
THERMODYNAMICS

1. For the reaction kyanite → andalusite (using the data in the table at the end of the problem set)

   a. Calculate the enthalpy of formation of kyanite and andalusite at 466 K and 10^5 Pa (1 bar).

   b. Calculate the enthalpy of the reaction. Is the reaction exothermic or endothermic?

c. Calculate the entropies of kyanite and andalusite at 466 K and 10^5 Pa.

d. Calculate the entropy change for this reaction

e. Calculate the free-energy change for this reaction. From the free energy value what can you conclude about this reaction under these conditions of temperature and pressure?

f. Calculate the change in free energy if the pressure is increased to 10^8 Pa At 466 K. Which mineral will be more stable under these new conditions? (Recall that 1 J = 1 Pa m^3)

2. The melting of a pure mineral can be written as a simple reaction. For diopside it is

$$\text{diopside}_{crystal} \rightarrow \text{diopside}_{liquid}$$

At 10^5 Pa (1 bar) diopside melts at 1665 K. If the S^o_{1665} of crystalline and liquid diopside are 532.2 and 619.6 J mol^{-1} K, respectively, and their volumes are, respectively, 0.06609 x 10^3 and 0.07609 x 10^3 m^3 mol^{-1}, calculate the melting point at 2 Gpa (20 kbar) using the Clapeyron equation. (Recall that 1 J = 1 Pa m^3)

3. The mineral jadeite, which is known to occur in metamorphic rocks formed at high pressures, can be related to two common low-pressure minerals by the reaction

$$\text{albite} \rightarrow \text{jadeite} + \text{quartz}$$

Use the data in the table at the end of the problem set to answer the following questions.

a. Balance the reaction and calculate the free energy of the reaction at 298 K and 10^5 Pa. Comment on the feasibility of the reaction under these conditions.

b. Repeat part (a), but for 600^{o}C and 10^5 Pa.

c. Calculate the pressure increases that would be needed at 298 and 873 K to bring the reaction to equilibrium.

d. How does the slope of this univariant line compare with the slope obtained from the Clapeyron equation and the data for 298 K and 10^5 Pa?

Table of Thermodynamic Data

Mineral	Volume (m^3 mol^{-1}) x 10^{-3}	ΔH_f^o (kJ mol^{-1})	S^o (J mol^{-1} K^{-1})	ΔG_f^o (kJ mol^{-1})	c_p^o coefficients a (J mol^{-1} K^{-1})	b x 10^{-3} (J mol^{-1} K^{-2})	c x 10^5 (J K mol^{-1})
Albite	0.10025	-3931.621	207.15	-3708.313	258.15	58.16	62.80
Andalusite	0.05153	-2576.783	92.88	-2429.176	172.84	26.33	51.85
Jadeite	0.0604	-3021.333	133.47	-2842.798	201.50	47.78	49.66
Kyanite	0.04409	-2581.097	83.68	-2430.720	173.19	28.52	53.90
Quartz	0.022688	-910.648	41.34	-856.239	46.94	34.31	11.30