Exam III Administered: Monday, November 14, 2022 24 points

For each problem part: 0 points if not attempted or no work shown,

1 point for partial credit, if work is shown,

2 points for correct numerical value of solution, if work is shown

Problem 1. (14 points)

Consider a mixture of four butanediol (C₄O₂H₁₀) isomers shown below.



Equilibrium coefficients, which relate mole fractions of components to one another, are given below:

$$K_{1,3-1,2}^{eq} = x_{1,3}/x_{1,2} = 0.665$$

$$K_{1,4-1,3}^{eq} = x_{1,4}/x_{1,3} = 0.740$$

$$K_{2,3-1,4}^{eq} = x_{2,3}/x_{1,4} = 0.542$$

The sum of the mole fractions is unity.

$$x_{1,2} + x_{1,3} + x_{1,4} + x_{2,3} = 1$$

- (a) Is this system of algebraic equations linear or nonlinear? (2 pts)
- (b) If linear, rearrange the problem as $\underline{Ax} = \underline{b}$ and identify $\underline{A}, \underline{x}$ and \underline{b} .

If nonlinear, rearrange the problem as
$$J\delta x = -R$$
 and identify $J, \delta x$ and R . (6 pts)

(c) Determine the composition of this mixture. (6 pts)

Problem 2. (10 points)

For the system described in problem 1, the equilibrium coefficients were evaluated at 300 K, using the relation

$$K_{1,3-1,2}^{eq} = exp\left(-\frac{\Delta G_{1,3-1,2}}{RT}\right) \text{ where } \Delta G_{1,3-1,2} = 1.018 \ kJ/mol$$

$$K_{1,4-1,3}^{eq} = exp\left(-\frac{\Delta G_{1,4-1,3}}{RT}\right) \text{ where } \Delta G_{1,4-1,3} = 0.750 \ kJ/mol$$

$$K_{2,3-1,4}^{eq} = exp\left(-\frac{\Delta G_{2,3-1,4}}{RT}\right) \text{ where } \Delta G_{2,3-1,4} = 1.526 \ kJ/mol$$

In Problem 2, you don't know the temperature but you do measure $x_{1,2} = 0.375$.

(a) Is this system of algebraic equations linear or nonlinear? (2 pts)

(b) Determine the temperature and the composition of the other three isomers. (8 pts)