Final Exam

Name _____ Student ID: _____

Exam Guidelines:

- Calculators and pencil/pens are permitted.
- Two sides of one note card (8.5x11" is allowed)
- All other materials, books, and cell phones should be zipped in your backpack.
- Show all your work and provide complete explanations to receive credit.
- Time = 110 minutes

Extra Space for your work below:

1. The enthalpy of mixing of acetone (AC) and cyclohexane (CH) is $\Delta h_{mix} = 6100 x_{AC} x_{CH}$.
    a. Estimate the partial molar enthalpy of mixing for cyclohexane in a mixture with 0.3 mol acetone and 0.2 mol acetone (8 pts).

    b. 0.3 mol acetone and 0.2 mol cyclohexane are mixed isothermally at 20 °C. Estimate the heat required to maintain the system at 20 °C (4 pts).

    c. The Antoine equation parameters for acetone and cyclohexane are shown on the table below. Estimate the saturation pressure of each component at 20 °C (6 pts).

	A	B	C
Acetone	4.42448	1312.253	-32.445
Cyclohexane	3.96988	1203.526	-50.287

Functional form of the Antoine equation: $log_{10}(P^{sat}[bar]) = A - \frac{B}{T[K]+C}$

d. The excess molar Gibbs free energy of the system can be approximated as $g^E = 4655\ x_{AC}x_{CH}$ (J/mol). Calculate the activity coefficients for acetone and cyclohexane in a mixture with 0.3 mol acetone and 0.2 mol cyclohexane. (8 pts)

e. Estimate the excess entropy of the system with 0.3 mol acetone and 0.2 mol cyclohexane (in J/K) (5 pts).

f. Estimate the excess molar entropy of cyclohexane (6 pts).

g. Estimate the molar entropy of cyclohexane (6 pts).

h. Assume that 0.3 mol acetone and 0.2 mol cyclohexane in the liquid phase are in equilibrium with a vapor phase. Estimate the pressure of the system (5 pts).

i. Calculate the vapor phase mole fractions of acetone and cyclohexane (4 pts).

2. Carbon monoxide and water react to form hydrogen and carbon dioxide. This reaction is called water gas shift (WGS) reaction:

$$CO + H_2O \rightarrow CO_2 + H_2$$

and is used to adjust the H_2:CO ratio of syngas prior to further reaction. For example, methanol synthesis requires a ratio of H_2:CO = 3.

In your refinery, you have a stream of 200 mol/min of CO flowing into a WGS unit, along with 150 mol/min of H_2 and 300 mol/min of steam (H_2O) at a pressure of 4 bar. Answer the following questions.

	$\Delta h_{f,298}^{o}$ (kJ/mol)	$\Delta g_{f,298}^{o}$ (kJ/mol)
CO	-110.53	-137.17
H_2O	-241.82	-228.57
CO_2	-393.51	-394.36
H_2	0	0

a. What is the standard enthalpy change of the reaction? (5 pts)

b. What is the equilibrium constant of the reaction at 298 K? (7 pts)

c. What temperature do you need to run the reaction, so as to achieve the required 3:1 H_2:CO ratio in the outlet? You may assume that the enthalpy change of the reaction is independent of temperature. (14 pts)

3: One of the reactions that takes place during the production of Portland cement, is the transformation of magnesium carbonate to magnesium oxide (lime), with production of CO_2 as a byproduct.

$MgCO_3 \rightarrow MgO + CO_2$

a. Without any calculations, do you think that the reaction is favored at low temperature or high temperature? Why? (6 pts)

b. The Gibbs free energies of formation of magnesium carbonate and magnesium oxide are -889.7 kJ/mol and -515.0 kJ/mol. The Gibbs free energy of formation of carbon dioxide is -395.6 kJ/mol. Calculate the equilibrium constant of the reaction at 800 K (6 pts).

c. Calcium carbonate and calcium oxide do not mix in the solid phase, but form separate solid phases. Knowing this, calculate the equilibrium partial pressure of CO_2 at 800 K (10 pts).