MASSACHUSETTS INSTITUTE OF TECHNOLOGY
20.110-5.60 Spring 2005

Exam #1, Friday October 7, 2005

WRITE YOUR NAME ON EVERY PAGE

NAME:____

RECITATION INSTRUCTOR:_______________________________

1._____/35
2._____/25
3._____/20
4._____/20

TOTAL:_____/100

This exam is closed book and closed notes, except that you are allowed to use one double-sided 8½" by 11" sheet of paper containing notes and equations. You are allowed to use a calculator. SHOW ALL YOUR WORK and CHECK YOUR UNITS!

R= 8.314 J K^{-1} mol^{-1}, R=0.08314 L bar K^{-1} mol^{-1}, T(K)=t(°C)+273.15

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1. (35 points)

Consider 1.0 moles of a monatomic ideal gas initially at T_1 = 300 K, p_1 = 1.0 bar, and V_1=25 L. The heat capacity at constant volume for this gas is $\overline{C}_V = \frac{3}{2}R$. The gas undergoes a closed cycle consisting of three processes. Careful with units!

(i) The gas first undergoes an irreversible adiabatic expansion against a constant external pressure of 0.5 bar to a final state at p_2 = 0.5 bar, T_2 = 240 K, and V_2 = 40 L.

(ii) Process (i) is followed by a reversible, constant volume heating back to the initial temperature T_1 = 300 K and a pressure p_3 = 0.625 bar.

(iii) The cycle is closed by a reversible isothermal compression back to the initial conditions (T_1=300 K, p_1=1 bar).

(a) (6 points) Compute ΔU, q, and w for process (i) (the first step). Make sure to provide units.

(b) (6 points) Give ΔU and ΔS for the complete cycle.

(c) (6 points) Compute ΔS for the gas for process (ii) (the reversible, constant volume heating). Make sure to provide units.

(d) (6 points) Compute ΔS for the gas for process (iii) (the reversible isothermal compression). Make sure to provide units.

(e) (6 points) Compute ΔS for the gas for process (i) (the irreversible adiabatic expansion). Make sure to provide units.

(f) (5 points) What is $\Delta S_{universe}$ for the complete cycle?

2. (25 points)

An aqueous solution of hydrogen peroxide (H_2O_2) consisting of 0.01 moles of H_2O_2 in 1 mole of H_2O is placed in a well insulated piston initially at 298 K and 1 bar. A small drop of the enzyme catalase (found in blood) is added to the solution, triggering the complete decomposition of the hydrogen peroxide according the reaction

$$H_2O_2\ (aq) = H_2O\ (\ell) + \tfrac{1}{2}\ O_2(g)$$

The pressure in the piston is kept constant at 1 bar during this adiabatic process. The final temperature of the solution is found to be 311 K.

	C_p(J K^{-1} $mole^{-1}$)
$H_2O_2(aq)$	89.1
$H_2O(\ell)$	75.2
$O_2(g)$	29.4

Assume all heat capacities are temperature independent for the purpose of this problem

(a) (5 points) What is ΔH for the adiabatic decomposition of 0.01 moles of hydrogen peroxide in solution at 1 bar (the ΔH for the experiment described)?

(b) (15 points) What is $\Delta\overline{H}^{o}_{rxn}$ for the isothermal decomposition of one mole of H_2O_2 at 298 K and 1bar (make sure to give units)?

(c) (5 points) Is the isothermal decomposition of H_2O_2 exothermic, endothermic or neither?

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3. (20 points)

Ribonuclease is a small protein that under certain conditions can fold in the following process

unfolded = folded

The heat for the folding process for a 500μL (1μL = 10^{-6} L) solution of the protein at a concentration of 1.0 μM (1μM = 10^{-6} mole/L) is measured at a constant pressure of 1 bar and at a constant temperature T = 30°C. The measurement is performed at two different values of pH.

reaction conditions	q (kJ)
1) pH = 1.13	-7.2×10^{-9}
2) pH = 2.5	-6.9×10^{-9}

a) (8 points) Give values for ΔH for the folding process for one mole of protein at 1 bar and T = 30 °C at both pH conditions.

b) (8 points) Values for ΔS for the folding process have also been tabulated:

reaction conditions	ΔS (kJ K^{-1} $mole^{-1}$)
1) pH = 1.13	-0.048
2) pH = 2.5	-0.044

Calculate ΔG for the folding process for one mole of protein at 1 bar and T = 30 °C at each pH value

c) (4 points) Is folding spontaneous at pH = 1.13 (p=1 bar, T=30 °C)? What about at pH = 2.5 (p=1 bar, T=30 °C)?

4. (20 points)

0.004 moles of liquid water (about 1 drop) at 1 bar and 373 K (the normal boiling point of water) is placed into a piston containing 0.04 moles of N_2 gas (about 1 liter) at 1 bar pressure and 373 K. The pressure is maintained at 1 bar and the temperature is maintained at 373 K. The drop of liquid water in the piston irreversibly and completely evaporates. The final state is 0.004 moles of water vapor mixed with 0.04 moles of N_2 gas at 1 bar and 373 K. Assume all gases are ideal. The process can be written as follows:

$$0.004\ H_2O(\ell,\ 1bar,\ 373K) + 0.04\ N_2(g,\ 1bar,\ 373K) = (0.004\ H_2O + 0.04\ N_2)_{mixed}\ (g,\ 1bar,\ 373K)$$

The following may be of use:

At the normal boiling point of water at 1bar and 373 K, the following process is reversible:
$H_2O(\ell,\ 1bar,\ 373K) = H_2O(g,\ 1bar,\ 373K)$ ΔH_{vap}=40,690 J/mole, ΔS_{vap}=109.1 J/mole

	C_p(J K^{-1} $mole^{-1}$)
$H_2O(\ell)$	75.2
$H_2O(g)$	33.6
$N_2(g)$	29.1

The entropy of mixing two ideal gases (A and B) is:
$\Delta S_{mix} = -nR(X_A \ln X_A + X_B \ln X_B)$,
where n is the total number of moles of gas and X_A and X_B are the mole fractions for gas A and B, respectively.

a) (12 points) What is ΔG for the complete process (the drop of water evaporating isothermally at 373 K in the presence of the nitrogen gas at a constant pressure of 1 bar)?

b) (4 points) Suppose that the nitrogen gas were not present in the piston. What would be ΔG for the isothermal evaporation of the drop of water in the piston at 1 bar and 373 K? Is it still an irreversible and complete evaporation?

c) (4 points) THIS PART IS ONLY IF YOU ARE DONE WITH ALL OF THE OTHER EXAM QUESTIONS, IT IS LONG BUT ONLY WORTH A FEW POINTS. Now take the process (the irreversible evaporation of the drop of water in the presence of nitrogen gas) and make both the initial and final temperatures at T = 298 K. What is ΔG now for the isothermal (T = 298 K) evaporation of the drop of water in the presence of the nitrogen gas? (Assume all heat capacities are temperature independent).