NAME: Notes JTG

Chemistry 130A, Prof. Groves

EXAM #1 Sept. 22, 2003

4 problems: 100 points

Please:
Write in pen
Do not use whiteout
Circle your answer clearly
If you use the back of the paper, be sure to mark clearly **in the space under the problem** where your work can be found.

Information:

Gas constant	$R = 8.3145\ J\ K^{-1}\ mol^{-1} = 0.08205\ L\ atm\ deg^{-1}\ mol^{-1}$
Boltzmann constant	$k = 1.38 \times 10^{-23}\ J\ K^{-1}\ mol^{-1}$
Conversion	L atm = 101.3 J

55.6 moles of water in 1 liter

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1. (25 pts total)
   a. (10pts) Indicate which of the following quantities are state variables:

[✓ P]

w X

[✓ PV]

$P_{ext}dV$ X

q_{rev} X

[✓ q_p] $(= H)$

[✓ $w + q$] $(= \Delta U)$

[✓ $w^2 + q^2 + 2wq$] $(= \Delta U^2)$

$w - q$ X $(= \Delta U - \underline{2q}$ ~ not state variable)

[✓ S]

b. (15pts) Consider a container of ideal gas, which can exchange heat and work with the surroundings, but nothing else. Indicate true or false for the following statements and provide a reason for your response (10 words or less for each). equation counts for 1 word).

The first and second laws of thermodynamics apply to this system.

True. 1^{st} + 2^{nd} laws always apply.

If the system energy increases by ΔU, the energy of the surroundings must decrease by ΔU.

True. Consequence of the first law

If the system expands *irreversibly* at constant T, $w = -q_{irr}$.

True. ConstanT implies $\Delta U = 0 = w + q \Rightarrow w = -q_{irr}$.

If the system expands *reversibly* at constant T, $\Delta S_{sys} + \Delta S_{surr} > 0$.

False. $\Delta S_{sys} = \frac{q_{rev}}{T}$ $\Delta S_{surr} = \frac{-q_{rev}}{T}$ $\Rightarrow \Delta S_{sys} + \Delta S_{surr} = 0$

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2. (25 pts Total) The antidepressant drug Prozac blocks the action of the neurotransmitter serotonin by competing for the binding site on the serotonin receptor.

Prozac-receptor → Prozac + receptor ΔH (20 °C) = 1200 kJ/mol

a) (10 pts) Which form has the lower internal energy, bound or unbound Prozac?

Bound form positive ΔH implies heat must be added to system

b) (15 pts) Calculate ΔH per mole for the reaction at 37 °C.

- Prozac-receptor complex molecular weight = 42,000 g/mol
- The difference in heat capacity for complexed and uncomplexed Prozac, $\Delta C_p = C_p(\text{complexed}) - C_p(\text{uncomplexed}) = 1.35$ J/(K gram)

$$\begin{tikzcd}
\underset{\text{complex}}{P\cdot R} \arrow[r, "\Delta H(37^\circ)"] \arrow[d, "\Delta H_1"'] & \underset{\text{uncomplexed}}{P + R} & 37\,^\circ C \\
P\cdot R \arrow[r, "\Delta H(20^\circ)"] & P + R \arrow[u, "\Delta H_2"'] & 20\,^\circ C
\end{tikzcd}$$

If you solve without reaction diagram:

$$\bigstar\quad \boxed{\begin{array}{l} \Delta H(T = 37°) = \Delta H(20°C) + \Delta C_p \Delta T \\ \qquad\qquad\qquad\qquad\qquad\quad \uparrow \\ \Delta C_p = C_p(\text{products}) - C_p(\text{reactants}) \\ \Delta C_p = -1.35 \end{array}}$$

Kirchoff's Law

$$\Delta H(37°C) = \Delta H_1 + \Delta H(20°C) + \Delta H_2$$

$$= C_p^{\text{complexed}}(20°C - 37°C) + \Delta H(20°C) + C_p^{\text{uncomplexed}}(37°C - 20°$$

$$= \Delta H(20°C) + \left(C_p^{\text{complexed}} - C_p^{\text{uncomplexed}}\right)(20°C - 37°C)$$

$$= \Delta H(20°C) + \Delta C_p(-17°C)$$

$$\therefore -17\text{ K} = \Delta T$$

$$= 1200\ \frac{\text{kJ}}{\text{mol}} + \left(1.35\ \frac{\text{J}}{\text{K}\cdot\text{g}} \cdot 42000\ \frac{\text{g}}{\text{mol}} \cdot \frac{1\text{ kJ}}{1000\text{ J}}\right)(-17\text{ K})$$

$$= \boxed{236.1\ \text{kJ/mol}}$$

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3. (25 pts Total) Consider a mixture of ideal gases consisting of molecule types A and B. The molecular weight of A is 30.0 g/mol.

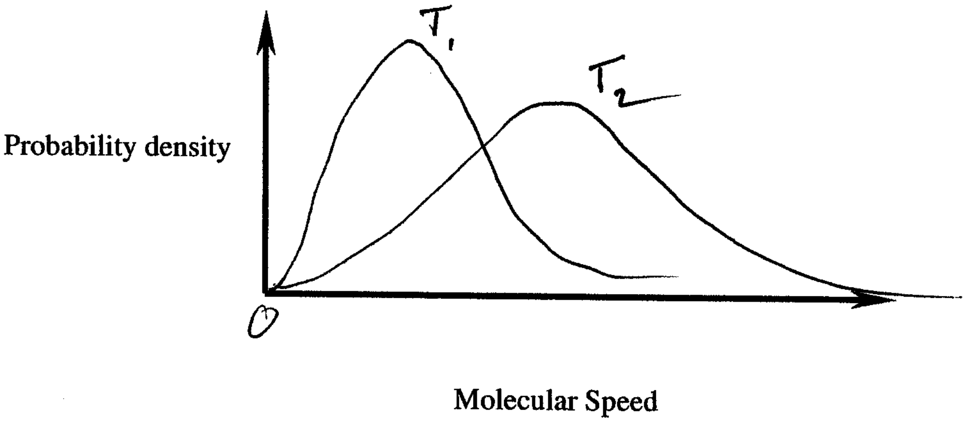
   a) (10 pts) What is the molecular weight of B if its root-mean-squared velocity is half that of molecule A. You may assume the two species of molecule are at the same temperature.

see solution from TA

$$\frac{V_{rms\,A}}{V_{rms\,B}} = 2 = \frac{\left(\frac{3k_BT}{M_A}\right)^{1/2}}{\left(\frac{3k_BT}{M_B}\right)^{1/2}} \quad . \quad 2 = \frac{(M_B)^{1/2}}{\sqrt{30}}$$

$M_B = 120\,g/mol$

   b) (15 pts) Draw a sketch of what you expect the molecular speed distribution functions to look like for molecule A at two different temperatures, T_1 and T_2, where $T_2 > T_1$. Draw two distribution functions, clearly label them, and provide a 15 word or less explanation for their differences.



Average speed (kinetic energy) is higher at higher temperature.

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4. (25 pts Total) The following problem concerns the expansion of an ideal gas from V_1 to V_2, under various conditions.

   a) (5 pts) Calculate the work (w) and heat (q_{rev}) for a reversible isothermal expansion. Express your answer as an equation in terms of V_1, V_2, T, and n. Explain how you obtained your result. → Equations can be used in explanation

   Reversible ⇒ $P_{ex} = P_{int} = \frac{nRT}{V}$

   $$w = -\int_{V_1}^{V_2} P\,dV = -\int_{V_1}^{V_2} \frac{nRT}{V}\,dV = -nRT\ln\left(\frac{V_2}{V_1}\right)$$

   Isothermal ⇒ $\Delta U = 0$ $q = -w = nRT\ln\left(\frac{V_2}{V_1}\right)$

   b) (10 pts) Imagine that the isothermal expansion takes place in a series of steps, each of which occurs rapidly enough that no molecules from the gas collide with the container walls while the walls are moving. Calculate w and q for this process, and explain any assumptions you make. Is it reversible?

   Work done when molecule collides with moving wall. Fast steps ⇒ $w = 0$ effectively $P_{ex} = 0$

   Isothermal ⇒ $\Delta U = 0$ $w = -q$

   $q = 0$

   Not reversible

   c) (10 pts) Imagine the expansion is adiabatic and occurs against a constant external pressure, P_{ex}. Calculate w and q. How does the temperature of the gas change? Express your answer for ΔT as an equation in terms of the relevant heat capacity and other quantities you may need. Explain any assumptions you make.

   $w = -\int P_{ex}\,dV = \boxed{-P_{ex}(V_2 - V_1)}$

   adiabatic ⇒ $\boxed{q = 0 \text{ for system}}$

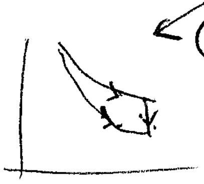
   However $\Delta U \neq 0$ since work done. ΔT is negative

   Determine ΔT from heat capacity, C_V ← why const volume?

   (+2) (see reverse)

   $\boxed{\Delta U = w = C_V \Delta T}$

   1pts $\Delta T = w/C_V = -P_{ex}(V_2 - V_1)/C_V$



Energy to do work comes from molecular KE

Break process into two steps.

1) Remove KE at constant volume to reach T_2

$\Delta T C_V$ is energy removed $= \Delta U$

2) isothermal expansion against P_{ext}

$w = -P_{ex} \Delta V$ but $w = -q$ this step

$\Delta U = 0$

~~Regardless of path~~