CH301 Week One

THINKING LIKE A CHEMIST

1. All matter is made of atoms – atoms are the building blocks of matter.
2. Chemists use electromagnetic radiation in indirect ways to "see" matter on the atomic scale.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. There are some basic principles and skills necessary to master in order to build a comprehensive understanding of chemical principles. Check your understanding of these principles and skills by stating the Law of Conversation of Mass in your own words and how it applies to our modern understanding of chemistry.

2. State the Laws of Definite Proportions and Multiple Proportions in your own words and explain how these laws support our modern understanding of the atomic nature of matter.

3. A 64 in ^{3} block of basalt weighs 116 ounces. Report this measurement as a density in units of g/cm^3. Can you estimate the density without using a calculator?

4. Without looking up the definitions of metric prefixes: Express 13.36 µm in centimeters; Express 0.076 kg in grams; Express 547 cm^3 in m^3.

5. Electromagnetic radiation displays wave-particle duality, which means that the light has both wave like and particle like properties. The interpretation of the photoelectric effect helped reveal this nature. Please sketch a diagram of the photoelectric effect experiment. Recall and explain the mathematical equation that relates the energy of the incident radiation to the potential energy of the electron and the resulting kinetic energy of the ejected electron.

6. Assuming that the maximum wavelength necessary to eject an electron from a metal surface is 240 nm, what would the work function be for the ejection of one mole of electrons from that metal surface?

7. Estimate the wavelength of a baseball weighing 5.15 oz (1 oz = 28.3g) thrown at 92 mph?

CH301 Week Two

THINKING LIKE A CHEMIST

1. All matter is made of electrons, protons & neutrons – elements consist of atoms with the same number of protons. The variation in properties of elements depends heavily on the electron configuration.
2. Subatomic and atomic properties cannot be explained using classical mechanics – rather, quantum mechanics can predict subatomic structure and energies.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. When energy is added to a pure element in the gas phase electromagnetic radiation is emitted. Please explain the origin of the emitted radiation.

2. Recall the Rydberg equation. Define each variable in the equation. As the potential energy of an electron in an atom increases the difference in energy between the electrons decreases. The empirically derived Rydberg equation accounted for this fact in what way? Use the Rydberg equation to calculate the difference in energy in electrons that could exist between energy levels 3 and 4 in a Hydrogen atom.

3. The Schrodinger equation was able to correctly predict the location in space where electrons were most likely to be found. What is meant by the terms "solutions" and "energies" in the context of the results from the Schrodinger equation?

4. The energies and solutions of the Shrodinger equation solved for the 1 electron hydrogen atom are labeled with quantum numbers, n, l and m_l.   Please define what each of these quantum numbers identifies.

5. Because each electron in an atom must have it's own unique set of quantum number, a fourth number needed to be added for atoms with more than one electron, what was that number and what is it's significance?

6. Electrons in an atom can be labeled using sets of possible quantum numbers or by using orbital notation. Write the orbital notion for Li and then state all the possible sets of four quantum numbers for each electron in Li.

7. Given the electron configuration and the orbital diagram for Se, answer the following questions. (In order to do this activity – you need to view a color copy – we will provide an online pdf in color.)

<u>Orbital Diagram for Se</u>   <u>Electron configuration for Se</u>

$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^{10}$, $4p^4$
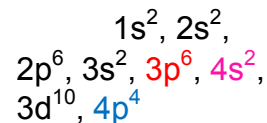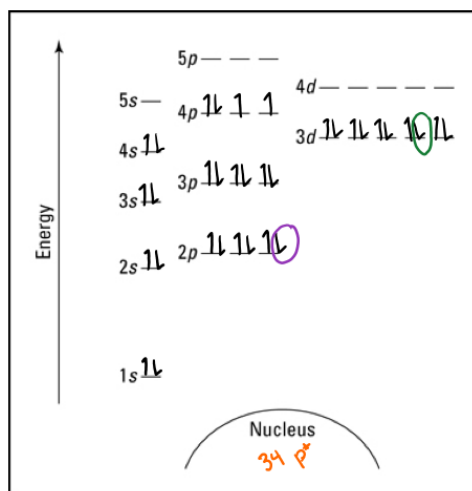
Questions

I. Orbital Diagrams: Where are the shells, sub-shells and orbitals on the orbital diagram? Circle and label each one on the diagram.

II. Electron Configuration and Orbital Diagrams
Where are the electrons in blue in the electron configuration on the orbital diagram? Circle them in blue on the orbital diagram.

Where is the electron circled in green in the orbital diagram in the electron configuration? What shell is this electron in? What sub-shell is this electron in?

III. Electron Configuration and Quantum Numbers

a. What are the possible quantum number sets for the electrons in pink on the electron configuration?

b. What are 3 possible quantum number sets for the electrons in red on the electron configuration? How many total possible quantum number sets are there for these electrons?

c. In orange on the electron configuration, circle the electrons with the quantum numbers: 2, 0, 0, -1/2 and 2, 0, 0, +1/2.

IV. Orbital Diagrams and Quantum Numbers

a. What are the possible quantum number sets for the electron circled in purple on the orbital diagram?

d. In light green on the orbital diagram, circle an electron with the quantum numbers: 3, 2, -2, -1/2.

V. Electron Configuration and the Periodic Table

a. Without looking at the periodic table, what row in the periodic table would you find Se? How do you know this?
b. Without looking at the periodic table, what block in the periodic table would you find Se? How do you know this?

CH301 Week Three

THINKING LIKE A CHEMIST

1. Location on periodic table matters – eg metals vs nonmetals grouped on table – based on subatomic architecture
2. Measure atomic radii & ionization energy and explain using ideas of nuclear charge and electron configuration

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. The atomic radii of lithium, sodium, potassium, and cesium are 243, 190, 167, and 298 pm, in no particular order. Match each element with its atomic radius. Explain your reasoning using the concept of effective nuclear charge.

2. The atomic radii of sodium, silicon, sulfur, chlorine, and argon are 111, 79, 88, 190, and 71 pm, in no particular order. Match each element with its atomic radius. Explain your reasoning using the concept of effective nuclear charge.

3. The first ionization energies for silicon, phosphorous, sulfur, and chlorine are 786.5, 1012, 999.6, and 1251.1 kJ/mol, respectively. Explain the exception to the general IE trend.

4. Write the electron configuration for vanadium using orbital notation and noble gas short hand method.

5. List a set of possible quantum numbers for an electron in the 3d orbital of vanadium.

6. Write the electron configuration for tellurium using orbital notation and noble gas short hand method.

7. Write the electron configuration for uranium using the noble gas short hand method.

8. Write the electron configuration for N^{3-} anion and Be^{2+} cation. Explain why the N^{3-} anion is larger than the Be^{2+} cation.

CH301 Week Four

THINKING LIKE A CHEMIST

1. Macroscopic properties of samples composed of ionic compounds versus covalent compounds vary based on the type of bonding that exists in those compounds, because the forces holding those compounds in the condensed phase depends on if the ion is the discrete unit or a molecule is the discrete unit in the sample.
2. Electrons arrange in the lowest energy state possible. This idea applies to both electrons in single atoms of elements and to electrons arranging to form bonds between atoms.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Explain, using a sketch and words, the potential energy well associated with the formation of a covalent bond. Include in your explanation why the well might be located at different points on the reaction coordinate axis and why the depth of the well might be different and what these differences imply in the context of bond strength and length.

2. Ionic compounds have varying melting points. Explain the factors that affect the melting points of ionic compounds.

3. Draw the Lewis structure for the following compounds: CF_2COCF_2 and CF_3CF_2OH.

4. Draw the Lewis structure for acetic acid, CH_3CO_2H. Confirm that your structure is the best structure based on the formal charge check.

5. Draw the Lewis structure for the acetate anion.

6. Draw the Lewis structure for N_2O.

7. Draw the Lewis structure for PCl_3 and PCl_5.

8. Draw the Lewis structure for BF_3 and BF_4^-.

CH301 Week Five

THINKING LIKE A CHEMIST

1. Bonding between atoms exists as a continuum between purely ionic and purely covalent.
2. Molecular shape depends on the distribution of all the electrons across the entire molecule. Understanding the fundamental fact that opposites attract and like charges repel, helps one to understand the distribution of negative charge across a molecule.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Study the molecule. How does one determine which atom is the "central atom"? How is the number of bonding regions around the central atom determined? How is the number of nonbonding regions around the central atom determined? What do these numbers of regions tell you about the electronic structure of the molecule?
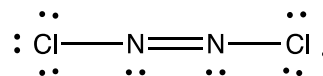

2. In what cases does the bond angle around a central atom deviate from a pure geometry, for example 117° rather than 120° for a pure trigonal planar geometry? What is the correlation between bond angles and number of bonding and nonbonding regions around the central atom of a molecule?

3. For the following molecules state the electronic geometry, the molecular geometry, and the valence bond hybridization around bold face atoms and state the polarity of the molecule:
   a. CH_2Br_2 f. $OC(NH_2)_2$
   b. $FCCF$ g. H_2CCH_2
   c. BH_3 h. AsF_3
   d. CH_3NH_2 i. SF_3H_3

5. State the electronic geometry, molecular geometry and VB hybridization around the atoms labeled in the following molecule:

6. Use orbital notation to show the VB hybridization of atomic orbitals that occurs when the sp hybrid orbital in HCCH is formed. Using the orbital notation show where all the valence electrons end up upon the formation of the triple bond.
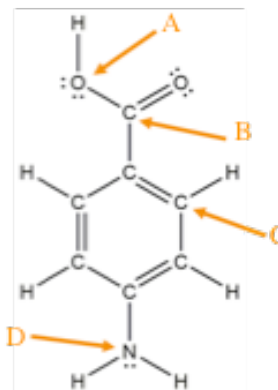
CH301 Week Six

THINKING LIKE A CHEMIST

1. Bonding in molecules can be explained using empirical and theoretical models. The theoretical models correctly predict the number and energies of molecular bonds. These theories include the purely empirical VSEPR theory, the mixed empirical and physical theory called VB theory, and the purely quantum mechanical MO theory. Chemists use all these different theories to help understand and predict chemical structures and reactivity.
2. Good molecular models allow the chemist to understand, explain and predict the macroscopic properties of different compounds.
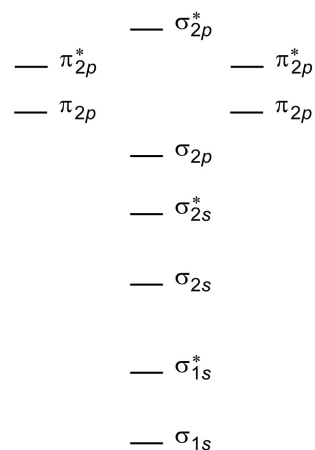
READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Fill in the Molecular Orbital diagram for CO.

Please state the bond order.

Please state whether this compound is expected to be paramagnetic or diamagnetic.

Please identify on the drawing the location of the HOMO and the LUMO.

$$\underline{\quad} \; \sigma_{2p}^*$$

$$\underline{\quad} \; \pi_{2p}^* \qquad \underline{\quad} \; \pi_{2p}^*$$

$$\underline{\quad} \; \pi_{2p} \qquad \underline{\quad} \; \pi_{2p}$$

$$\underline{\quad} \; \sigma_{2p}$$

$$\underline{\quad} \; \sigma_{2s}^*$$

$$\underline{\quad} \; \sigma_{2s}$$

$$\underline{\quad} \; \sigma_{1s}^*$$

$$\underline{\quad} \; \sigma_{1s}$$

2. From the line drawing write the correct molecular formula.
State the valence bond hybridization around the "central" atoms where indicated with an arrow. In addition state the electronic geometry and molecular geometry around each of these "central atoms". State the number of pi bonds. Circle the regions containing delocalized bonds. Circle the polar bonds. State the polarity of the molecule.
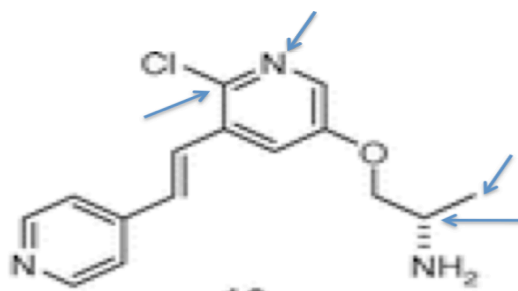
CH301 Week Seven

THINKING LIKE A CHEMIST

1. The macroscopic properties of ideal gases depend on microscopic behaviors of gases. Early scientists observed the macroscopic properties of P, T, V and amount of gas, and from these observations speculated as to the molecular properties of gases resulting in a "small particle" model of gases. A mathematical model called the kinetic molecular theory supported empirically derived "small particle" model.
2. Empirically derived gas laws can be used to accurately predict behavior of ideal gases.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. In August 1783, Jacques Charles poured liquid sulfuric acid on solid iron metal to produce hydrogen gas and solid iron(III) sulfate. He funneled the hydrogen gas into a large balloon to produce the first hot air balloon. The balloon traveled 21 km away to a nearby city, at which the local peasants were so scared that they destroyed his beloved science project with their pitchforks and knives.
   a. Write the corresponding chemical equation.
   b. If Jacques Charles treated 174 L of sulfuric acid with excess iron at STP, what volume of hydrogen gas was produced?
2. In December 1783, Jacques Charles and Nicolas-Louis Roberts traveled in the first-manned hot air balloon. They reached a height of 1800 ft, where they observed a pressure of 94.19 kPa and a temperature of 11 °C. At this point, they realized that they only had 10 g of Fe remaining. They quickly calculated that they would need exactly 6.14 L of hydrogen gas to return safely back to the ground. Did they survive?
3. Later that day, Jacques Charles traveled alone to a height of 3000 ft, where he experienced incredible ear pain. It hurt him so badly that he vowed to never ride in a hot air balloon again.
   a. Using sketches to support your argument, why did Jacques Charles experience this pain at 3000 ft, but not at ground level? Please describe this situation both macroscopically and microscopically.
   b. Not only did Jacques Charles experience horrible ear pain, but he also found it very difficult to maintain high oxygen levels. At 3000 ft, the % O_2 of air decreased from 20.9% to 18.6%., and the temperature dropped to 9 °C with a pressure of 90.81 kPa. Compare the average kinetic energies and the average velocities of nitrogen, oxygen and argon molecules at this altitude. No calculations are necessary to answer this question.
   c. At this altitude, the composition of nitrogen is still 78%. What are the partial pressures of oxygen and nitrogen at 3000 ft? Please answer in atm.

CH301 Week Eight

THINKING LIKE A CHEMIST

1. The ideal gas law breaks down when gases are exposed to conditions which violate the postulates of the KMT, in particular at pressure high enough and temperatures low enough to allow substantial intermolecular interactions that ultimately lead to condensation and solidification.
2. Macroscopic properties of liquids can be explained using the microscopic ideas of intermolecular forces.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. From a molecular perspective, what is changing as the pressure on a gas increases while the temperature remains constant? In theory, as the pressure increases the volume approaches 0. How is this possible? What factor can account for this elimination of volume in the ideal gas law? As pressure increases and temperature decreases, gas molecules get close enough and are slowed down enough to impart attractive forces. What factor can account for this elimination of elastic collisions? Draw a small particle sketch to show microscopically the conditions that lead to condensation.
2. Propanol ($CH_3CH_2CH_2OH$) and Glycerol ($CH_2OHCH_2OHCH_2OH$) are both considered to be alcohols. While they both exist as liquids at room temperature, their liquid properties are different. Explain how you expect the properties to be different. Support your answer with a full molecular explanation, including the types of IMFs.
3. Given the following data provide a "molecular view" description of the trend in boiling points based on all intermolecular forces for the given molecules. In your answer include whether or not each compound exists as a solid, liquid or gas at room temperature, draw the 3-D structure of each, and state the types of IMF that exist in each compound.

Compound	Boiling Point, Melting Point
CHF_3	191 K, 26 K
$CHCl_3$	334 K, 210 K
$CHBr_3$	415 K, 319 K
CHI_3	490 K, 396 K

CH301 Week Nine

THINKING LIKE A CHEMIST

1. Macroscopic properties of solids can be explained using the microscopic ideas of intermolecular forces.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Fully describe (macroscopic and "molecular" view with words and pictures) the two solids I_2 (mp = 386 K) and KI (mp = 959 K).

2. To fully prepare for this test you should be able to explain the following:

   I.   Describe the difference/similarities between a polar bond and a polar molecule.

   II.   Describe the differences/similarities between a bond and an intermolecular force. Include in your description the term "hydrogen bond" in the context of IMFs.

   III. Describe the differences/similarities between polar and polarizable.

   IV.   Describe the differences/similarities between molecule and molecular solid and covalent solid.

   V.   Explain the relationship between boiling point, vapor pressure and the Boltzmann distribution of KE's for a liquid at given temperature in the context of IMFs.

CH301 Week Ten

THINKING LIKE A CHEMIST

1. The First Law of Thermodynamics states that energy of the universe is conserved. A practical application of this big idea in the study of chemistry is that the energy that is released or absorbed across a chemical or physical changes must either be coming from or going into the system that is undergoing change.

2. The internal energy of a chemical system is the sum of all the potential and kinetic energy of that system. Any changes in the quantity of internal energy must occur when energy leaves or enters the systems in the form of heat or work.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Acetylene (C_2H_2) combusts in oxygen to form carbon dioxide and water. Assume that you combust 5 g of C_2H_2 in excess oxygen, how much work would have been done by this process?

2. Balance the following reaction of hydrazine with methanol. Calculate the work done.
   $$N_2H_2(l) + CH_3OH(l) \rightarrow CH_2O(g) + N_2(g) + H_2(g)$$

3. If the work done on a system is 5.7 kJ, and the external pressure is equal to 3.5 atm. Is the volume of the system increasing or decreasing?

4. Substances have different heat capacities. Differentiate between the terms heat capacity, molar heat capacity and specific heat capacity. Which of the following substances would you suppose has the higher specific heat capacity water or benzene (C_6H_6)? Justify your answer.

5. A gas in a cylinder was placed in a cooler and lost 500 kJ of heat. If the cylinder decreased in volume from 1846 mL to 548 mL against an internal pressure of 750 Torr during the process, what is the change in internal energy of the gas in the cylinder?

6. Calculate the heat necessary to increase the temperature of ethanol from 20 °C to 40 °C. The heat capacity of ethanol is 2.42 J/g °C.

CH301 Week Eleven

THINKING LIKE A CHEMIST

1. The amount of heat flowing between the system and its surroundings can be macroscopically observed and measured using a calorimeter. The flow of energy can be modeled using the thermodynamic state ΔH, which is a measure of q_p or ΔU which is a measure of q_v.

2. The enthalpy of a chemical system is a measure of it's chemical potential energy. In the case of phase changes we interpret the ΔH as the change in the PE of IMFs and in the case of chemical changes we interpret the ΔH as the change in the PE of the reactants versus the products. The ΔH is a state function and as such is path independent.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Acetylene (C_2H_2) combusts in oxygen to form carbon dioxide and water. Estimate the enthalpy of combustion of acetylene using bond energies data. Sketch a graph of enthalpy versus reaction path for this exothermic reaction. Comment on the the PE of the products versus the PE of the reactants?

2. Calculate the enthalpy of combustion of one mole of C_2H_2 using heats of formation data found on the course gchem site using your personal wireless device.

Single Bond Energies (kJ/mol of bonds)

	H	C	N	O	S	F	Cl
H	436						
C	413	346					
N	391	305	163				
O	463	358	201	146			
S	347	272	—	—	226		
F	565	485	283	190	284	155	
Cl	432	339	192	218	255	253	242

Multiple Bond Energies (kJ/mol of bonds)

C=C 602	C=N 615	C=O 799
C≡C 835	C≡N 887	C≡O 1072
N=N 418	O=O 498	N≡N 945

3. At constant pressure, use the change in enthalpy and the work to find the change in internal energy for the combustion of 4 g C_2H_2.

4. 4 g of acetylene was combusted in a bomb calorimeter that had a heat capacity of 3.51 kJ/C for the device and contained 2000 g of water (C = 4.184 J/g C). What is the expected temperature change in such a calorimeter given the complete combustion of the 4 g of the fuel.

CH301 Week Twelve

THINKING LIKE A CHEMIST

1. The Second Law of Thermodynamics states that all spontaneous changes are accompanied by an increase in universal entropy. Entropy is defined as the dispersal of energy. So as long as the dispersal of energy is increasing in the universe the change will be spontaneous.
2. ΔS_{sys} will accompany every chemical and physical change. It is important to be able to differentiate between ΔS_{sys} and ΔS_{surr} so you can fully understand the fundamental nature of spontaneous change.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

1. Let's look at a process with which we are all familiar: Ice melting in a glass of water. Imagine you start with a glass that has **36 g** of solid ice. The initial temperature of the ice is 0 °C. If you leave this glass in a room that has a constant temperature of 25 °C, the ice will *spontaneously* melt and you will end up with all liquid water at 25 °C. Here we will calculate the entropy change for the process of the ice melting and increasing in temperature to 25 °C. First identify what the system and surroundings are. (what are they composed of, what is their temperature, etc…) Often it is helpful to make a sketch or diagram.

2. Now identify what the initial and final states of the system are. Again a diagram, equation, or sketch can be helpful. You should break this down into two steps: ice melting, then water warming up.

3. Now look at the energy change for this process. Does energy flow into or out of the system? If so, as heat or work?

4. Given that $\Delta_{fus}H° = 6.02$ kJ mol^{-1} and that the heat capacity for water is 4.184 J g^{-1} °C^{-1} . How much heat flows into the system for this process (in kJ)?

5. What is the change in entropy for the melting of the ice? What is the change in entropy for the melting of the water? What is the change in entropy for the system?

6. Did heat flow into or out of the surroundings during this change?
7. What is the entropy change for the surroundings?
8. What is the entropy change for the universe for this process?
9. The answer to part 8 is extensive (this for the 36 g of solid ice that melts in this process). What is the entropy change per mole of solid ice that melts under these conditions?

The equation $\Delta S = q_{rev}/T$ holds for reversible heat flow. However, during a chemical change the heat flow is not reversible. Therefore, we need another way to determine the change in entropy for the system such that we can predict the spontaneity of chemical change. The Boltzman definition allows a method for determining the standard molar entropy a compound, because $S = k_B \ln \Omega$. When there is only one microstate, $S = 0$. This occurs at 0 K in a perfect crystal, thus there is an absolute value for entropy. The standard molar entropies for elements and compounds have been computed and are available in tables. One can use these values to determine the change in entropy for chemical change! Remember that entropy is a state function, and the change in the state function only depends on the final condition minus the initial condition.

1. Use the following tabulated data:

$S°(H_2)g = 131$ J/K mol

$S°(O_2)g = 205$ J/ K mol

$S°(H_2O)l = 70$ J/K mol

to determine the change in entropy for the combustion of 1 mole of hydrogen.

2. Use the following tabulated data:
    $\Delta H_f°(H_2O)l = -286$ kJ/mol

to determine the change in entropy for the surroundings for this change under standard conditions.

3. Use your answers from 1 and 2 to determine the change in entropy for the universe, and predict if this change is spontaneous under standard conditions.

CH301 Week Thirteen

THINKING LIKE A CHEMIST

1. Gibbs Free Energy is a concept invented to incorporate the ΔS_{surr} into state function of a defined system. ΔG depends on both the ΔH and the ΔS of the system. Energetically favorable process is one in which the ΔH decreases across the change and the ΔS increases across the same change. ΔG is a convenient way to predict spontaneity of change!
2. $\Delta G = 0$ indicates that the state is at a minimum energy state and such change either forward or reverse is not spontaneous.

READINESS ASSESSMENT QUIZ – CHALLENGE YOURSELF

Consider the following PHYSICAL CHANGE:

$$N_2(liq, 77K) \longrightarrow N_2(gas, 298K)$$
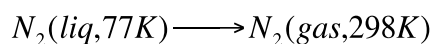
and the following THERMODYNAMIC DATA for N_2 :

$$\Delta H^0_{vaporization} = 5.56 \ \text{kJ mol}^{-1}$$

$$C(N_{2gas}) = 29.1 \ \text{J K}^{-1}\text{mol}^{-1}$$

1. $T_b = 77 \text{ K}$ $\qquad\qquad T_{surr} = 298 \text{ K}$

    1. How much heat is absorbed during this change given 4 moles of N_2?
    2. What is the work for this process (assuming the initial volume of the liquid is zero) assuming that you are starting with 4 moles of liquid?
    3. What is the change in internal energy for this process?
    4. What is the change in enthalpy for this process?
    5. What is the change in entropy of the system for this process?
    6. What is the change in entropy of the surrounding for this process?
    7. What is the total change in entropy (change in entropy of universe) for this process?
    8. Does the thermodynamic calculation predict the observation that this process is spontaneous?
    9. Determine the change in Gibbs free energy for this process at 298K.
    10. Is this change spontaneous at 350 K? Is it spontaneous at 77K? Is it spontaneous at 50 K? Please explain.