### CHEM 103 Summary of Semester

Lecture Notes May 9, 2006 Prof. Sevian





#### Announcements

 The final exam is scheduled for Monday, May 15, 8:00-11:00am
 It will NOT be in our regularly scheduled lecture hall (S-1-006). The final exam location has been changed to Snowden Auditorium (W-1-088).



#### More announcements

Information you need for registering for the second semester of general chemistry

- If you will take it in the summer:
  - Look for chem 104 in the summer schedule (includes lecture and lab)
- If you will take it in the fall:
  - Look for chem 116 (lecture) and chem 118 (lab). These courses are co-requisites.
- If you plan to re-take chem 103, in the summer it will be listed as chem 103 (lecture + lab). In the fall it will be listed as chem 115 (lecture) + chem 117 (lab), which are co-requisites.
  - Note: you are only eligible for a lab exemption if you previously passed the course.



#### Agenda

- Molecular orbital theory (see lecture notes from last Thursday)
  - Energy level diagrams for simple diatomic molecules
  - Bonding vs. antibonding orbitals → bond order predictions
  - Other predictive features: excited states, paramagnetism
  - Compare MO theory to VB theory for same molecule
- Summary and perspective of entire semester



#### **Course Review**

Overarching principle: Chemists view nature at three levels.

- 1. Macroscopic
  - Matter that comprises everything
  - Properties of materials
- 2. Particle level
  - Structure of matter
  - Energy that governs interactions of particles
- 3. Symbolic
  - Ways of representing behavior of matter

Each level provides information

#### Matter is made of atoms



- Atoms are comprised of protons, neutrons and electrons.
- All the different kinds of atoms are cataloged in the Periodic table.
- The atom is very small. The area of a nucleus is 1/100,000<sup>th</sup> the area of an atom. The atom is mostly empty space.
- The protons define the identity of an atom.
- The numbers of neutrons can vary, giving rise to isotopes.
- The number of electrons can vary:
  - Neutral atom: same quantity as protons
  - Negative ion: more electrons than protons
  - Positive ion: fewer electrons than protons



#### Matter is made of atoms

- Different atoms have different masses, due chiefly to differing numbers of protons and neutrons (which weigh much more than electrons).
- Quantities of matter can be measured either by numbers of particles (in the case of atoms or molecules) or units (in the case of ionic compounds) in a sample of the material, or by the mass of the sample. It is possible to convert between these two measurements of quantity of matter using molar mass.
   For example,

 $18.5 \ g \ Al \times \frac{1 \ mol \ Al}{26.98 \ g \ Al} = 0.686 \ mol \ Al$ 

• In a compound, atoms are present in exact ratios of moles, so percent composition by mass is also fixed.

#### What does % composition mean?



Note: These are approximate atomic masses, for the purpose of demonstrating % composition. When actually calculating % composition, use the values from the Periodic Table.



% Composition by Mass

fraction C = 
$$\frac{2 \times 12}{60}$$
 = 40.%  
fraction H =  $\frac{4 \times 1}{60}$  = 6.7%  
fraction O =  $\frac{2 \times 16}{60}$  = 53%

#### Composition of a Compound



 What is the composition by mass of acetic acid (CH<sub>3</sub>COOH)?

%C = 
$$\frac{24.02}{60.05} \times 100\% = 40.00\%$$

$$\% H = \frac{4.032g}{60.05g} \times 100\% = 6.714\%$$

%O =  $\frac{32.00g}{60.05g} \times 100\% = 53.29\%$ 

Check: 40.00 + 6.714 + 53.29 = 100.00%



Recall how to get: Molar mass = 60.05 g/mol



#### % Composition to Empirical Formula

Analysis of a particular compound shows that it is composed of X% carbon, Y% hydrogen, and Z% oxygen.What is the compound's empirical formula?

#### $M \land S S (grams) \implies M \land O \sqcup E S (mol)$



#### % Composition to Empirical Formula



Analysis of a particular compound shows that it is composed of 73.14% carbon, 7.37% hydrogen, and the remainder is oxygen. What is the compound's empirical formula?

$$\frac{73.14 \text{ g C}}{12.01 \text{ g}} \times \frac{1 \text{ mol C}}{12.01 \text{ g}} = 6.089 \text{ mol C}$$

$$\frac{7.37 \text{ g H}}{1.008 \text{ g}} \times \frac{1 \text{ mol H}}{1.008 \text{ g}} = 7.31 \text{ mol H}$$

$$\frac{19.49 \text{ g O}}{16.00 \text{ g}} \times \frac{1 \text{ mol O}}{16.00 \text{ g}} = 1.218 \text{ mol O}$$

$$= 1.218 \text{ mol O}$$

$$= 1 \times 5 : 1.200 \times 5 : 0.2000 \times 5$$

$$= 5 : 6 : 1$$
so, empirical formula is C<sub>5</sub>H<sub>6</sub>O<sub>1</sub>



#### Matter is made of atoms

- Atoms are conserved in all processes (except nuclear decay).
  - All stoichiometry calculations are based on this principle: In a chemical change, the number of atoms of each kind that enters the reaction must equal the number of atoms of each kind that exit the reaction.
    - This means you must balance chemical reactions first before doing stoichiometry calculations.
  - The maximum amount of product in a reaction is determined by the least reactant that is available (the most reactant that can be used in a process is equal to the least reactant available).



#### Writing Net Ionic Equations



- 1. Start with the balanced reaction, written with phases
- 2. Identify ions in aqueous solution, ionic solids that precipitate, and any molecules on both sides of the arrow
- 3. Cross out any spectator ions
- 4. What's left is the net ionic equation



Net reaction: two I<sup>-</sup> ions + one Hg<sup>2+</sup> ion  $\rightarrow$  one unit of HgI<sub>2</sub> ppt

2 I<sup>-</sup> (*aq*) + Hg<sup>2+</sup> (*aq*)  $\rightarrow$  HgI<sub>2</sub> (*s*)



### A Stoichiometry Calculation

If 0.252 g of calcium chloride were present in the reactant calcium chloride solution, how many grams of silver chloride should be formed if all the calcium chloride is used up?







The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

Strategy:

- Empirical formula means ratio of moles
- Need to know moles of C and moles of H
- Get moles of C from mass of CO<sub>2</sub>
- Get moles of H from mass of H<sub>2</sub>O
- Determine empirical formula of butane from ratio of moles C:H

#### **Combustion Analysis Example**



The combustion of 0.5320 g butane (in a lighter) produces 1.6114 g of carbon dioxide and 0.8247 g of water.

(a) What is the empirical formula for butane?

Start				End
1.6114 g CO <sub>2</sub>	1 mol CO <sub>2</sub>	1 mol C	_	0.036614 mol C
	44.011 g CO <sub>2</sub>	1 mol CO <sub>2</sub>	=	
Start				End
0.8247 g H <sub>2</sub> O	1 mol H <sub>2</sub> O	2 mol H	_	0.09153 mol H
	18.02 g H <sub>2</sub> O	1 mol H <sub>2</sub> O	=	

<sup>(</sup>a) If butane contains only C and H, what is the empirical formula for butane?





The combustion of 0.5320 g butane (in a lighter) produces 0.4028 g of carbon dioxide and 0.8243 g of water.

(a) What is the empirical formula for butane?

#### Ratio of Moles C : Moles H

 $\frac{0.036614 \text{ mol C}}{0.036614} : \frac{0.09153 \text{ mol H}}{0.036614} = 1: 2.5 = 2:5$ 

Empirical formula is C<sub>2</sub>H<sub>5</sub>





#### Continuation of the same problem...

(b) A different analytical procedure indicated that 9.153 × 10<sup>-3</sup> moles of butane were present in the original sample of butane. What is the molecular formula for butane?

Strategy:

- Start with empirical formula from part (a)
- Use mass and moles to calculate molar mass of butane
- Find out how many empirical units are in butane
- Molecular formula of butane is same factor × empirical formula



# (b) A different analytical procedure indicated that 9 153 × 10

(b) A different analytical procedure indicated that  $9.153 \times 10^{-3}$  moles of butane were present in the original sample of butane. What is the molecular formula for butane?

Molar mass is measured in g/mol

Molar mass of butane =

0.5320 g butane

- = 58.12 g/mol

 $9.153\times10^{\text{-3}}$  moles of butane

#### **Combustion Analysis Example**



(b) A different analytical procedure indicated that  $9.153 \times 10^{-3}$  moles of butane were present in the original sample of butane. What is the molecular formula for butane?



### Elements display periodicity



- The organization of the Periodic table is based on mathematical solutions (called wave functions, or orbitals) to the Schrodinger equation for hydrogen.
- The Periodic table is a model of how chemists understand the electronic structure of atoms.
- The periodic nature of the elements in the Periodic table gives rise to trends in physical properties of the elements.

## Spectroscopy provides evidence for wave behavior of electrons and light



Macroscopic observations

- When energy enters atoms, atoms give off light at discrete wavelengths (line emission spectrum)
- Line emission is fingerprint of an element
- Entire periodic table at http://javalab.uoregon.edu/dcaley/elements/Elements.html

Particle level explanation

- Electrons are so small that their quantum mechanical properties become important (Heisenberg uncertainty principle)
- Electrons can reside in various different quantum mechanical potential energy states, only one of which is the lowest energy ground state
- See http://www.avogadro.co.uk/light/bohr/spectra.htm

Symbolic representation (mathematical model)

#### Implications of Quantum Mechanical Model



- Energy of electron is quantized (only certain states are allowed)
- Due to Heisenberg uncertainty principle, it is impossible to identify both position of electron and its energy, so if energy is given by the S equation, then equation can only predict probability of locating electron within a given region of space (orbital), also called electron density
- Orbitals (solutions to S equation) are specified mathematically by quantum numbers: n, l, m<sub>l</sub>, which are interdependent

## 3 quantum numbers specify solutions to the Schrodinger equation (called orbitals)



- Principal quantum number ( $n = 1, 2, 3, ...\infty$ ) Specifies energy of the electron Sometimes called "shell", in reference to Bohr model  $E_n = -Rhc/n^2$  (same as Bohr/Rydberg)
- Angular momentum quantum number (l = 0, 1, 2, ..., n-1) Specifies 3-D shape of probability map of electron density Sometimes called subshell Often coded by letters corresponding to different values for ll = 0, 1, 2, 3, ... corresponds to *s*, *p*, *d*, *f*, ...
- Magnetic quantum number ( $m_l = 0, \pm 1, \pm 2, \pm 3, \pm l$ ) Orientation of orbitals (mathematical solutions to S equation) within a subshell

### What Orbitals Are

- Electron cloud pictures
- Probability density describing where electron is located
- Proportional to the square of the wave function with specific quantum numbers (wave function symbolized by Greek letter ψ)
- Think of a bird at a bird feeder, and a time-lapse photo





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### **Electron Configurations**



#### Periodic Table Structure





#### **Ionization Energies of Elements**

The energy required to remove the most weakly bound electron from an atom or ion.

Data from H. Sevian et al, Active Chemistry

#### Chemical bonds form when electrons pair



- Bonding between atoms can be modeled in two ways: valence bond theory and molecular orbital theory.
- In valence bond theory, atomic orbitals on individual atoms hybridize to form hybrid (mixed) orbitals of equal energy. When an orbital has one electron in it, it can form a bond by overlapping with an orbital on a different atom that also has one electron in it. The overlap of the hybrid atomic orbitals creates a bonding orbital with a pair of bonding electrons in it.
- In molecular orbital theory, all atomic orbitals on all atoms in the molecule combine mathematically to form molecular orbitals that spread out in space over the entire molecule. When electrons are in bonding orbitals, bonds form. When electrons are in antibonding orbitals, they cancel bonds.

## Two kinds of bonding lead to two kinds of compounds



Ionic Compounds

- Contain ions
- Held together by electrostatic attraction between + and – ions: these attractions called ionic bonds
- Ionic formula: simply the ratio of ions present in order for the compound to be neutral, cannot separate a unique unit

#### Molecular Compounds

- Do not contain ions
- Atoms within molecules held together by covalent bonds in which electrons from both atoms are attracted to the nuclei of both atoms in a bond
- In a molecular solid, one molecule held to the next by weaker forces of attraction
- Molecular formula: can separate unique molecules

#### Writing Chemical Formulas and Naming Chemical Compounds



- Formulas to names
  - Determine whether ionic or molecular
  - If ionic, name = (positive ion) (negative ion)
  - If molecular, use prefixes
  - Acids next week
- Names to formulas
  - Translate the formula
  - If ionic, find ions, then balance charges
  - If molecular, read the prefixes
  - Acids next week



## The shapes and sizes of particles determine the properties of materials



- Molecular shape is determined by the underlying geometry of the bonding orbitals.
- Molecules can be either symmetric or not symmetric.
- If a molecule is not symmetric, and if it has at least one polar bond, then the molecule is polar.
- (Polar molecules interact with each other differently than nonpolar molecules do.)

## All behavior of particles can be explained by the attractions/repulsions between unlike/like charges



- Forces of attraction and repulsion are explained by the Coulomb model, where the force is proportional to two things:
  - 1. The magnitudes of the charges that interact.
  - 2. The distance separating the charges.
- Changes in matter are due to the energetics dictated by the forces in matter. Energy is conserved in all changes.
  - Two atoms that are bonded have lower potential energy than two atoms separated, so when atoms bond they give off energy.
- Energy changes are path independent.





### Solubility: Physical Principles



- The force of attraction between oppositely charged ions is proportional to the magnitude of the charges of those ions.
- During dissociation, oppositely charged ions in the solid phase are separated from each other and dissolved in water.
- This suggests that:
  - If a salt is composed of highly charged ions, it is not very soluble.
  - If a salt is composed of ions with lower charges, it is probably soluble.
- General rule to use as a starting point: any salt involving a +1 cation or a -1 anion is *likely* to be soluble.

Acknowledgment: Blake, B. (2003) J. Chem. Ed. 80, 1348.

#### Calorimetry

How much heat is released if the temperature rises from 23.3°C to 34.6°C when 4.50 g of NaOH are added to 100.0 g of water?



#### Problem Solving Strategy

 $q_w = m_w C_w \Delta T_w$ where  $\Delta T_w = temp$  change of H<sub>2</sub>O  $q_{sys}$  is opposite of  $q_w$ 

<u>Given information</u> Mass of water = 100.0 g Mass of NaOH = 4.50 g Temperature of water before = 23.3°C Temperature of water after = 34.6°C

 $C_{water} = 4.184 \text{ J/g} \cdot \text{K}$ 

104.5 g total

Beaker image: core.ecu.edu/chem/chemlab/ equipment/ebeaker.htm



