

Chapter R

Chemistry 130 - Fall 2019

Chapter R: Measurement and Calculations in Chemistry (L1)

Pre-reading assignments: Chapter R

Learning Goals for Chapter R

sig fig

- Report values to appropriate number of significant figures using rules for calculations and uncertainty in measurement
- Solve problems systematically using unit conversions and dimensional analysis
- Understand and calculate density of substances
- Classify matter from mixtures to atoms and distinguish physical and chemical changes

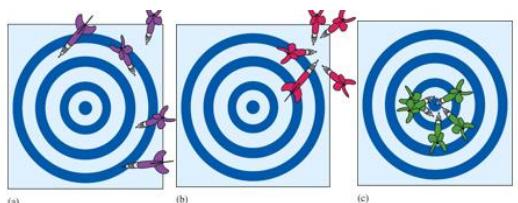
R.1 Units of Measurement

- **Measurement:** a quantitative observation consisting of a number and a scale (unit)
- Fundamental SI units: see periodic table packet for base units and prefixes
- A nickel has a mass of 0.005 kg. What is the mass in g? _____
- $1 \text{ dm} = 10 \text{ cm}$; $1 \text{ dm}^3 = \underline{\hspace{2cm}} \text{ cm}^3$

R.2 Uncertainty in Measurement

- An estimated digit is called uncertain.
- A measurement always has some uncertainty. E.g. 1 mL and 1.00 mL
- Record the certain digits and the first uncertain digit (the estimated number).
- Example:

Precision and Accuracy – Figure R-4



precise &
accurate

R.3 Significant Figures and Calculations

Significant Figures – Rules for counting significant figures

1. Nonzero : always count

2. zero : ① leading \times

② middle ✓

③ trailing 100 100. 1.00

(Count when has decimal point) 1 3 3

Significant Figures – Rules for calculations with correct significant figures

- Multiplication and division

the # of sigfigs is the least precise

$$\frac{4.56}{3} \times \frac{1.4}{2} = 6.384 \rightarrow \frac{6.4}{2}$$

- Addition and subtraction

the # of decimal is the least precise

$$\begin{array}{r}
 12.1 \\
 18.2 \\
 \hline
 1.013 \\
 \hline
 31.123
 \end{array}
 \quad \downarrow \quad 31.1$$

- Rounding

based on 5

Exercise R.26e: Perform the mathematical operation and express the result to the correct number of significant figures

$$\frac{9.875 \times 10^2 - 9.795 \times 10^2}{9.875 \times 10^2} \times 100 \text{ (exact)} =$$

$$\begin{aligned}
 & \frac{0.080}{9.875} \times 100 = 8.10127 \times 10^{-3} \times 10^3 \\
 & = 8.1 \times 10^{-1}
 \end{aligned}$$

R.4 Learning to Solve Problems Systematically

1. Where are we going? Goal
2. How do we get there?
3. What do we know? Given

R.5 Dimensional Analysis

- Use when converting from one system of units to another
 - Use the conversion factor that relates the two units.
 - Cancel unwanted units
 - Multiply to give the quantity with the desired units.

Practice: An iron sample has a mass of 4.50 lb. What is the mass of this sample in grams? (1 kg = 2.2046 lb; 1 kg = 1000 g)

Therefore: lbs of iron \rightarrow kg of iron \rightarrow g of iron

$$4.50 \text{ lb} \rightarrow \frac{4.5}{2.2046} \text{ kg} \rightarrow \frac{4.5}{2.2046} \times 10^3 \text{ g}$$

$$= 2.04 \times 10^3 \text{ g}$$

$$65 \text{ mile/h}$$

$$1 \text{ mile} = 5280 \text{ ft}$$

$$3ft = 1 \text{ yard}$$

$$1 \text{ mile} = 1760 \text{ yards}$$

$$1760 \text{ yards/h}$$

$$32 \text{ yards/s}$$

R.6 Temperature

- 3 systems: Fahrenheit, Celsius, Kelvin

$$T_C = T_K - 273.15 \quad T_F = T_C \times \frac{9^{\circ}\text{F}}{5^{\circ}\text{C}} + 32^{\circ}\text{F}$$

R.7 Density

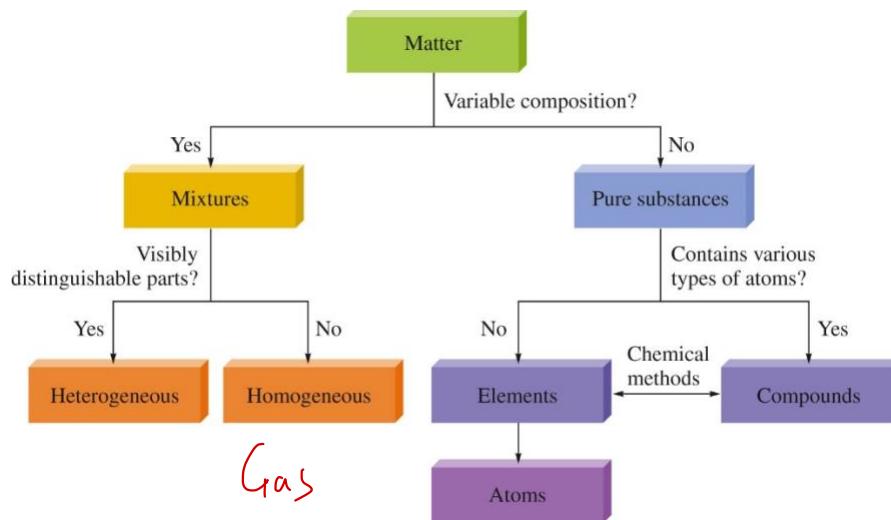
$$D = \frac{\text{Mass of a substance}}{\text{volume}}$$

Common units:

Practice (R.61): Given the following information, which of the following has the greater mass: 75 mL of copper or 1.0 L of benzene?

Substance	Density
Liquid benzene	0.880 g/mL
Solid copper	8.96 g/mL

R.8 Classification of Matter



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Chemical change

- Given substance becomes a new substance with different properties and chemical composition
- Example:

Physical change

- Change in form, not chemical composition
- Example:

Separation of mixtures by physical change or physical property

- e.g. distillation, filtration, chromatography

Practice (R.72) A teaspoon of magnesium filings and a teaspoon of powdered sulfur are placed together in a metal beaker. Would this constitute a mixture or a pure substance?

Suppose the magnesium filings and sulfur are heated so they react with each other, forming magnesium sulfide. Would this be a mixture or pure substance? Why or why not?

R.9 Energy and R.10 The Mole: See textbook.

These sections will be expanded upon for Exam 2 and 3 content.

Energy: Ability to do work or to produce heat.

- Work – force acting over a distance.
- Heat – energy that flows from one object to another because of a temperature difference.
- SI unit is the Joule. $1\text{ J} = 1\text{ kg m}^2/\text{s}^2$

Mole: A unit for counting atoms and molecules

$$1\text{ mole} = 6.022 \times 10^{23} \text{ items}$$

$$1\text{ dozen} = 12 \text{ items}$$

Online HW : OWL v2

12 assignments 2 drop

Lecture.

Lecture :

Read chapter early

Solve problem during class
[periodical table

Discussion:

Work on problem In group

quizzes

3 Exams

2 + 1

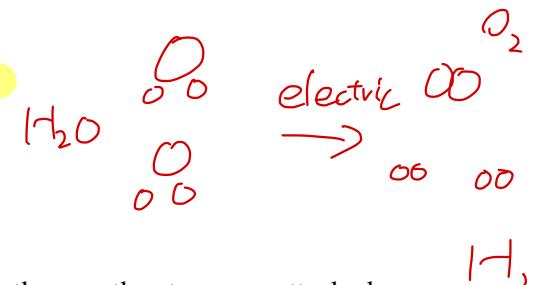
Chapter 1

Chapter 1: Chemical Foundations (L2-3)

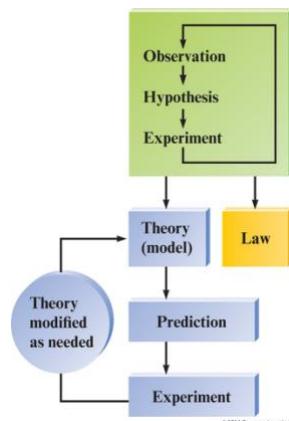
Pre-reading assignments: Chapter 1

Learning Goals for Chapter 1

- Recognize the difference between a scientific theory, model, and law
- Apply the fundamental chemical laws to experimental observations and calculations: conservation of mass, definite proportions, multiple proportions
- Recall the four postulates of Dalton's Atomic Theory and describe aspects that are disproven and aspects that are still considered valid
- Describe historical experimental set-up, observations, and models used to characterize the atom
- Write the nuclide symbols for atoms and ions
- Determine the number of protons, neutrons, or electrons in an atom or ion given some atomic information

1.1 An atoms-first approach*Atoms versus molecules**Diatomeric molecules: Elements that naturally possess two atoms**Chemical reaction:* One substance changes to another by reorganizing the way the atoms are attached to each other**1.2 The scientific method (Figure 1-4)**

Natural law: summary of observed phenomenon

Theory (model): attempt to explain *why* phenomenon occurs**1.3 The Early History of Chemistry***Not on exam. Read for fun!***1.4 Fundamental chemical laws**

Law of conservation of mass

Law of definite proportions *LDP*

A sample of H_2SO_4 contains 2.02 g of hydrogen, 32.07 g of sulfur and 64.00 g of oxygen. How many grams of sulfur are present in a second sample of H_2SO_4 containing 7.27 g of hydrogen?

Law of multiple proportions

$$7.27 \times \frac{32.07}{2.02}$$

The following data were collected for several compounds of nitrogen and oxygen. Show how these data illustrate the law of multiple proportions.

LMP: the ratios of the masses of N combining with 1 g O in each pair of compounds should be small whole numbers.

Compound	Mass of N that combines with 1 g of O
A	
B	
C	

Compound B has the formula NO. What are the formulas of compounds A and C?

1.5 Dalton's Atomic Theory (1808)

- Elements made up of atoms
- Atoms of an element are identical *X (not true) Isotopes*
- Chemical compounds form when atoms of different elements combine
 - A compound always has same relative numbers and types of atoms
- Chemical reactions involve reorganization of atoms—changes in way they're bound
 - Atoms are not changed in chemical reaction *X ionization*

Joseph Guy-Lussac's Observations

ionization

Avogadro's hypothesis: At the same temperature and pressure, equal volumes of different gases contain the same number of particles.



1.6 Early experiments to characterize the atom

About the atom:

- Atoms contain negatively charged particles called electrons.
- The mass of the electron is $9.11 \times 10^{-31} kg$
- The charge on the electron is $1.60 \times 10^{-19} C$
- Atoms contain a small, dense center of positive charge.

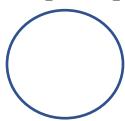
How do we know?

Observation
experiments

The electron – JJ Thomson

Cathode ray tube

Proposed plum pudding model



Determined:

1. Negative particles in ALL atoms.
2. atoms are all neutral

The charge and mass of an electron – Robert Millikan

Charged oil drop experiment

Determined the magnitude of the charge on an electron

Calculated the mass of an electron

The nuclear atom – Ernest Rutherford

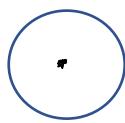
Used alpha particles (α) - Possess a charge twice that of the electron, with the opposite sign

Metal foil experiment

Expected results

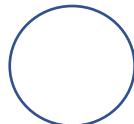


Observation and model



1.7 Modern view of atomic structure: An Introduction

Composition of an atom:



Isotopes

same number of [protons] but different number of [neutrons]

Example: isotopes of sodium

Nuclide symbol:

Ions: charged atoms

- Electron removed:

- Electron added:

Practice

atomic



Symbol	# of protons	# of neutrons	# of electrons	Net charge
Ba ²⁺	56	81	54	2 ⁺
Br ⁻				
³ H				
	8	9	8	0
	3	4	3	0

Chapter 2

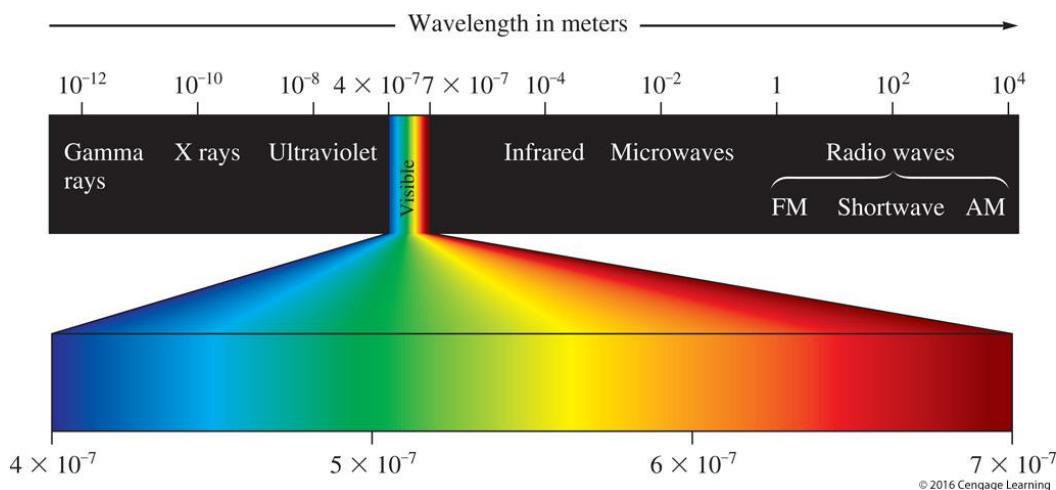
Chapter 2: Atomic Structure and Periodicity

Pre-lecture reading assignment: Chapter 2

Chapter 2 Learning Goals

- Explain the dual nature of light and the experiments and observations which led to that conclusion
- Calculate energy, frequency, and wavelength of electromagnetic radiation
- Explain the photoelectric effect and calculate work functions and electron energies
- Explain electronic transitions and atomic line spectra
- Describe the Bohr model and its limitations
- Calculate the energy change for electron transitions using the Bohr model
- Apply the concepts of standing waves and probability distribution to atomic orbitals in the quantum mechanical model
- Apply the quantum number rules to any given electron to determine correct sets of quantum numbers
- Correlate quantum numbers to orbital shapes and energies
- Describe the effect of multiple electrons on radial probability for an electron in a polyelectronic atom
- Draw orbital diagrams and write electron configurations for a given atom, applying Hund's Rule, the Pauli Principle, and the Aufbau Principle
- Write and recognize the electron configurations for transition metal exceptions Cr and Cu
- Identify the valence electrons, noble gas core, and valence electron configuration for a given atom
- Explain the trend of effective nuclear charge and how it influences the trends of atomic radius, ionization energy, and electron affinity
- Predict relative atomic radii, ionization energies, and electron affinities for a set of atoms and/or ions based on periodic trends
- Explain exceptions to the trends for ionization energy and electron affinity using energy level diagrams (e.g. Be and B ionization energy, N and O ionization energy, and N + 1 electron is unstable)

2-1 Electromagnetic radiation



wave

$$c = \nu\lambda \quad \lambda: \text{ wave length}$$

ν : frequency

$$\lambda = \frac{3.9979 \times 10^8 \text{ m/s}}{3.84 \times 10^{14} \text{ s}^{-1}} = 1.04 \times 10^{-6} \text{ m.}$$

2-2 The nature of matter (the dual nature of light)

Waves diffract

Particles vs. waves

Simulate Thomas Young's Experiment: phet.colorado.edu/en/simulation/legacy/wave-interference

Diffraction patterns

Destructive constructive



The photoelectric effect

Simulate photoelectric effect: <https://phet.colorado.edu/en/simulation/legacy/photoelectric>

Key observations of the photoelectric effect

When $\nu < \nu_0$,

No electron emitted.

When $\nu > \nu_0$,

low energy emit

When $\nu > \nu_0$,

Wave or particle?

Observation	Explained by waves	Explained by particles
Diffraction		
Photoelectric effect		

Quantization: energy is limited to certain values

Max Planck observed that energy can be gained or lost only in whole-number multiples of $h\nu$, where h is Planck's constant. The energy change for a system can be represented by:

$$\Delta E = n\hbar\nu$$

Albert Einstein proposed that light (electromagnetic radiation) is composed of particles (quanta) called photons.

The energy of each photon is proportional to its frequency:

$$E_{\text{photon}} = h\nu$$

Photoelectric effect explained by Einstein

- Threshold energy to remove an electron = $E_0 = h\nu_0$

- When $\nu > \nu_0$, the excess energy is kinetic energy (KE):

$$\begin{aligned} KE_{\text{electron}} &= \frac{1}{2}mv^2 = h\nu - h\nu_0 \\ &= h\nu - \phi \end{aligned}$$

Practice: X-ray photons, each with an energy 2.3816×10^{-16} J, strike copper foil. The work function (minimum energy to remove an electron) of copper is 7.5×10^{-19} J. What is the kinetic energy of the reflected electron?

$$C = (h\nu - \phi) = 2.3816 \times 10^{-14} \text{ J}$$

If solid calcium has a photoelectric threshold of 11.14×10^{14} Hz, will an electron be ejected upon radiation with a light beam of frequency 2.0×10^{12} s⁻¹?

The de Broglie relation

Practice: Compare the wavelengths of an electron and a baseball. ($\hbar = 6.626 \times 10^{-34}$ J·s; and the unit Joule is: mkg·s⁻²)

Electron $m_e = 9.11 \times 10^{-31}$ kg $v = 3.00 \times 10^6$ m/s $\lambda =$

Baseball $m = 0.145$ kg $v = 26.8$ m/s (60 mph) $\lambda =$

2-3 The atomic spectrum of hydrogen

Continuous spectrum: all wavelengths

Line spectrum/emission spectrum: only specific wavelengths (only certain energies)

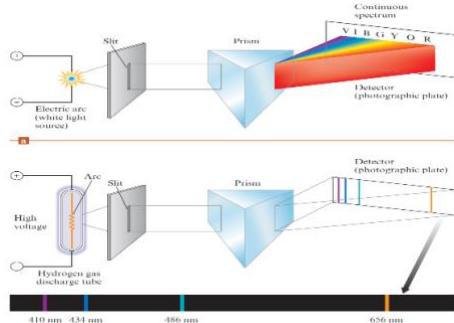
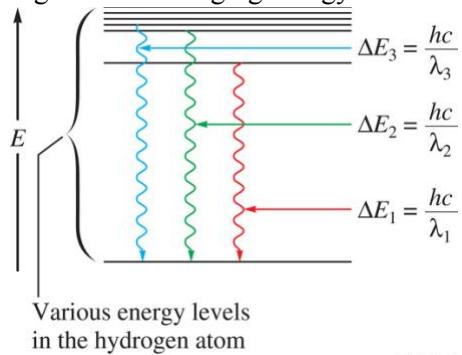


Figure 2.7:

How does the emission spectrum of hydrogen support the idea of quantized energy levels?

Figure 2-8: Changing energy levels emits a photon of light



2-4 The Bohr Model

- The electron of the hydrogen atom travels in certain allowed circular orbits.
- Available energy levels can be expressed as:

$$E = -2.178 \times 10^{-18} \text{ J} \left(\frac{Z^2}{n^2} \right)$$

- Lowest possible energy state is called: _____
- Importance of the Bohr model:
 - o The model correctly fits the quantized energy levels of the hydrogen atom
 - Only circular orbits allowed in this model.
 - o As the electron becomes more tightly bound, its energy becomes more negative relative to the free electron
 - The free electron is at infinite distance from the nucleus
 - As the electron is brought closer to the nucleus, energy is released from the system (more negative relative to the free electron)
- Limitations of the Bohr Model:
 - o Only works for atoms with 1 electron
 - o Circular orbitals are incorrect

Electronic transitions in the Bohr model for the hydrogen atom

$$\Delta E = E_f - E_i \quad \boxed{\Delta E = -R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)} \quad R_H = 2.178 \times 10^{-18} \text{ J, Rydberg constant}$$

Practice: Calculate the wavelength of light emitted for the transition from an electron in the $n=5$ level to the $n=3$ level.

$$0.15488 \times 10^{-18} \text{ J} = \frac{hc}{\lambda}$$

\curvearrowleft

2-5 The quantum mechanical model of the atom

Standing waves: ends are fixed (the wave does not travel) and it vibrates with only certain allowed frequencies

Hydrogen electron vibrates in this defined space and only whole number n values are allowed.

Erwin Schrödinger and Quantum Mechanics: Where are we *most likely* to find an electron?

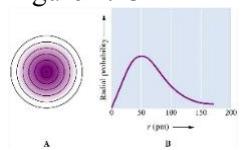
Schrödinger's calculated positions in 3D space called *wave functions*, ψ (amplitude of a standing wave)

- There are many possible wave functions for a given electron. They are called *orbitals*.
- The ψ_2 gives us the probability of finding the particle within a region of space $\hat{H}\psi = E\psi$

The physical meaning of a wave function: *Radial probability distribution*

- The ψ_2 gives us the probability of finding the particle within a region of space
- Example: Probability distribution for hydrogen 1s orbital in three-dimensional space.

Figure 2.13



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Heisenberg Uncertainty Principle

- It is impossible to know both position *and* momentum of a particle at a given time

$$\Delta x \cdot \Delta(mv) \geq \frac{h}{4\pi}$$

2-6 Quantum numbers

Quantum mechanics: each electron described by 4 quantum numbers:

- Principal quantum number

n integral

size

- Angular momentum quantum number

$l \sim n-1$

shape

subshell

- Magnetic quantum number

$+l \sim -l$

0	1	2	3
s	p	d	f

- _____

Practice: For principal quantum level $n = 5$, determine the number of allowed subshells (different values of l), and give the designation of each.

Practice: Explain why each of the following sets of quantum numbers is not permissible for an orbital.

a. $n = 0, l = 2, m_l = -2$

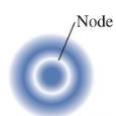
b. $n = 3, l = 3, m_l = 0$

c. $n = 2, l = 1, m_l = +2$

d. $n = 4, l = 2, m_l = -3$

2-7 Orbital shapes and energies

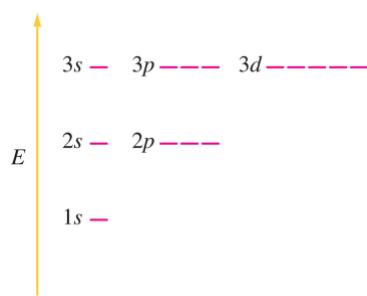
Nodal surface:



Atomic orbitals:

- s
- p
- d
- f

Degenerate orbitals



Summary of the hydrogen atom

- QM model: electron is a standing wave.
- Orbitals describe the possible energies and spatial distribution of the electron
- We can picture orbitals in terms of probability distributions (electron density maps)
- H has many orbitals. Ground state is 1s but the electron can be excited to higher-energy orbitals if energy is added to the atom.

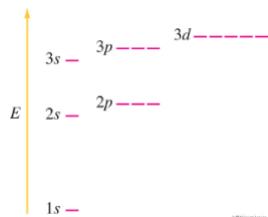
2-8 Electron spin and the Pauli principle

The Spinning Electron – the ~~4_{th}~~ quantum number (insert on the list of quantum numbers in 2-6)

Pauli exclusion principle states that in a given atom no two electrons can have the same set of four quantum numbers.

2-9 Polyelectronic atoms

Polyelectronic atom energy levels – orbitals with same n are no longer degenerate! (Zumdahl & Zumdahl Figure 2-22)



Penetration effect:

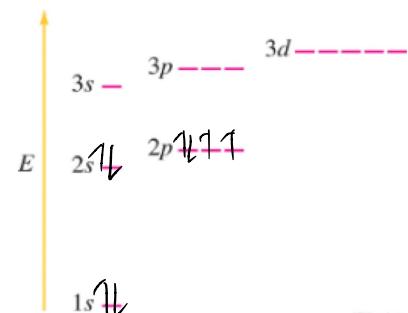
2-10 not covered, not on exam

2-11 The Aufbau principle and the periodic table

Aufbau principle:

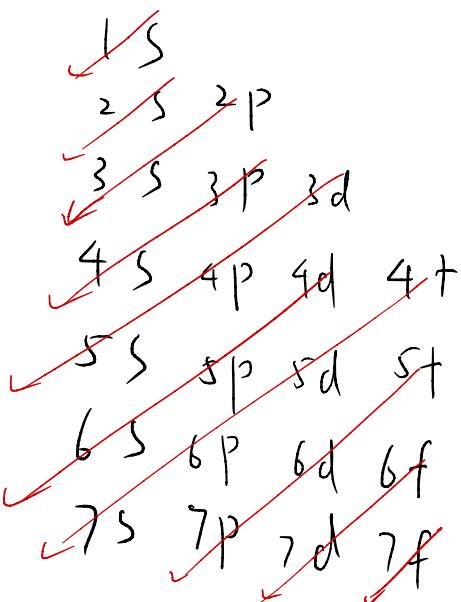
Hund's Rule: the lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate orbitals

$1e^-$	H: $1s^1$	<table border="1"> <tr><td>1</td></tr> </table>	1	<table border="1"> <tr><td></td></tr> </table>		<table border="1"> <tr><td></td></tr> </table>		
1								
$3e^-$	Li: $1s^2 2s^1$	<table border="1"> <tr><td>1</td></tr> </table>	1	<table border="1"> <tr><td>1</td></tr> </table>	1	<table border="1"> <tr><td></td></tr> </table>		
1								
1								
$6e^-$	C: $1s^2 2s^2 2p^2$	<table border="1"> <tr><td>1</td></tr> </table>	1	<table border="1"> <tr><td>1</td></tr> </table>	1	<table border="1"> <tr><td>1</td></tr> <tr><td>1</td></tr> </table>	1	1
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Electron configuration examples:

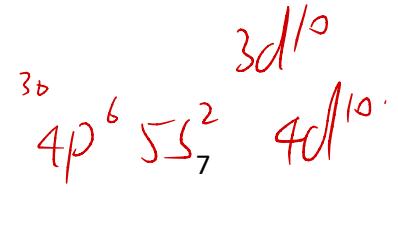
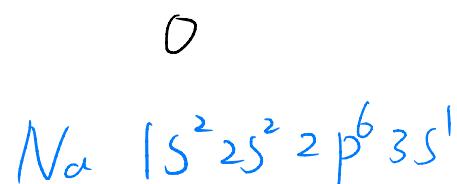
Noble gas configuration



Valence electrons

in the outermost level

Core electrons



Groups in the periodic table

- Main group elements

 $1A \sim 3A$

- Transition metals

- Valence:

- Exceptions to memorize:

- Lanthanides and Actinides

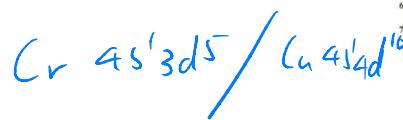
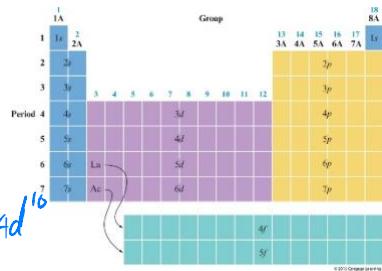


Figure 2-29 The orbitals being filled



$16e^-$ sulfur S

$1s^2 2s^2 2p^6 3s^2 3p^4$

$48e^-$ Cd

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^{6-2}$
 $4f^{10}$

[Kr] $5s^2 4d^{10}$

Practice:

Write the ground state electron configuration for iron ($Z = 26$).

$1s^2 2s^2 2p^6 3s^2 3p^6 Ar 4s^2 3p^6$

Write the ground state electron configuration for potassium.

$Ar 1s^1$

2-12 Periodic trends in atomic properties

Effective nuclear charge (Z^*)

proton numbers

decrease

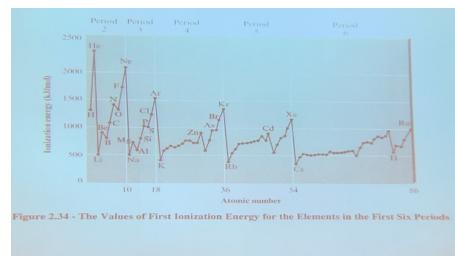
Atomic radius

increase ↗ O O O O

Practice: Predict the trend in radius for the following ions: Be^{2+} , Mg^{2+} , Ca^{2+} , and Sr^{2+}

Ionization energy

$Be^{2+} < Mg^{2+} < Ca^{2+} < Sr^{2+}$

Exceptions to trend in first ionization energy (I_1)

Rb < Na < Be
Sr < Se < Ne
Fe < P < O

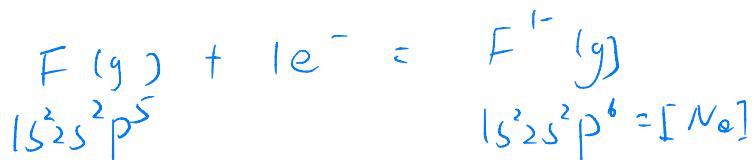
Practice: Consider atoms with the following electron configurations. Which atom has the largest first ionization energy, and which one has the smallest second ionization energy?

$1s_2 2s_2 2p_6$

$1s_2 2s_2 2p_6 3s_1$

$1s_2 2s_2 2p_6 3s_2$

Electron affinity

**2-13 The properties of a group: the alkali metals**

Special names for main groups in the periodic table

1A Alkali Metals (active)

2A

7A

8A

which is least stable

1A Alkali

Ionization energy ↓

radius ↑

Density ↑

Ch 1:

- Intro to Chemical Law

Law of multiple proportion

- Early atomic experiments

Ch. 2 development of quantum mechanics

- electromagnetic radiation

- nature of light

- emission spectrum ($n=1$)

B_ohr model

Quantum mechanical of atom

Orbitals.

n, l, m

Chapter 3

Chapter Outline

CHEM 130 FA 19

Dr. Albright

Chapter 3 – Bonding: General Concepts (L9 – L13)

Pre-lecture reading: Chapter 3

Chapter 3 Learning Goals

- Compare and contrast ionic and covalent bonding
- Compare ionic bond energies using Coulomb's law
- Compare polarity of covalent bonds based on electronegativity differences in atoms by apply the periodic trend
- Predict formulas and names of ionic compounds
- Predict relative ionic radii by applying the periodic trend of ionic radius
- Calculate and compare magnitudes of lattice energies
- Use energy changes for reactions in a multi-step process to calculate the energy change for one reaction or the overall energy change
- Calculate the energy change for a reaction using average bond energy values
- Draw appropriate Lewis structures for molecules
- Apply the duet rule, octet rule, and known exceptions to drawing Lewis structures
- Draw and recognize resonance structures for a given molecule
- Calculate formal charges and apply that to determining the best Lewis structure for a given molecule
- Apply nomenclature rules to name ionic and molecular compounds given the formulas

3-1 Types of chemical bonds

Representation of Molecular Structures

Chemical bond vs Molecule

chemical bond
molecule

Molecules can be represented using:

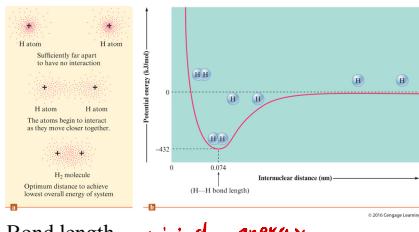
- Chemical formula
- Structural formula
- Space-filling model: Ball and stick method:

Ionic bond

$$E = (2.31 \times 10^{-19} \text{ J} \cdot \text{nm}) \left(\frac{Q_1 Q_2}{r} \right)$$

Zumdahl & Zumdahl Figure 3-2:

Charge of atoms
negative - release - attractive



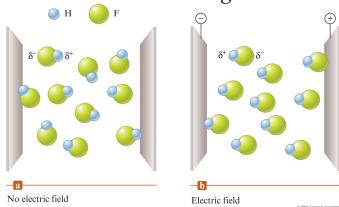
Bond length *minimized energy*

Covalent bond

atoms share electrons

Polar covalent bond

Zumdahl & Zumdahl Figure 3-3:



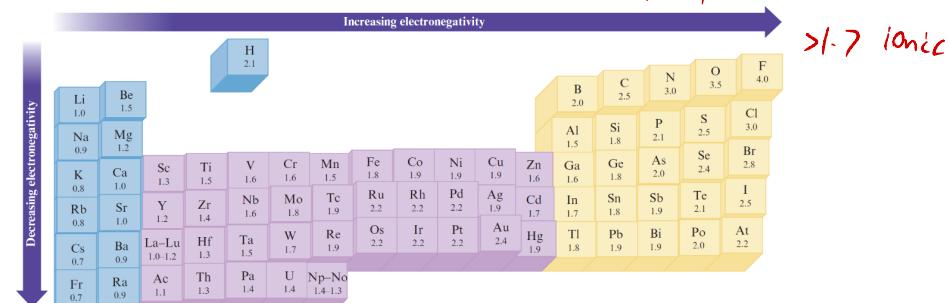
3-2 Electronegativity: ability of an atom in a molecule to attract shared electrons to itself

0.9 - 0.4 *covalent*

2.4 - 1.7 *polar-covalent*

>1.7 *ionic*

Zumdahl & Zumdahl Figure 3-4:

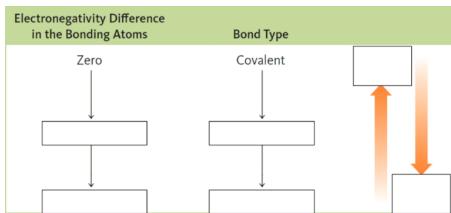


Determining values of electronegativity

Bond character: Zumdahl & Zumdahl Table 3-1:

expected H-X energy

$$= \frac{H-H \text{ bond energy} + X-X \text{ bond energy}}{2}$$



Concept check:

- If lithium and fluorine react, which has more attraction for an electron? Why?
- In a bond between fluorine and iodine, which has more attraction for an electron? Why?

Clicker (3.41)

Hydrogen has an electronegativity value between boron and carbon and identical to phosphorus. With this in mind, rank the following bonds in order of decreasing polarity:



3-3 Ions: Electron configurations and sizes

Electron configuration of compounds

noble gas configuration



Predicting Formulas of Ionic Compounds

- Chemical compounds are always electrically neutral

Practice: What are 5 ions that have the electron configuration of neon?

Sizes of ions

- Ion size influences structure and stability of ionic solids
- Size is determined by the distance between ion centers
- Factors that influence ionic size:

Practice: Choose the largest ion in each of the following groups:

- Li^+ , Na^+ , K^+ , Rb^+ , Cs^+

- Ba^{2+} , Cs^+ , I^- , Te^{2-}

Isoelectronic ions

~~End exam 1 content~*~*

3-4 Energy effects in binary ionic compounds

Lattice energy: The change in energy when separated gaseous ions are packed together to form an ionic solid

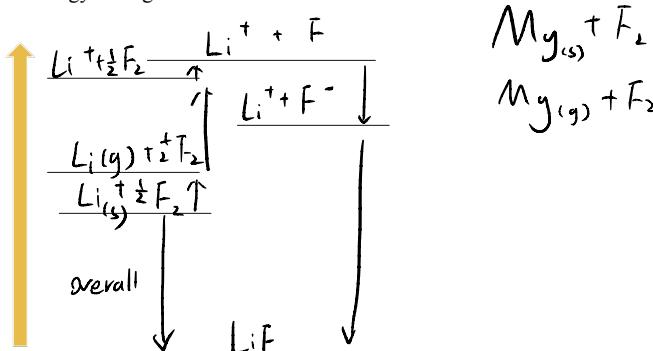
Lattice energy calculations

$$k \left(\frac{Q_1 Q_2}{r} \right)$$

Born – Haber Cycle

Formation of an ionic solid

Example: Energy Changes in the Formation of Lithium Fluoride



Example question:

Use the following data for magnesium fluoride to estimate ΔE for the reaction: $\text{Mg}(s) + \text{F}_2(g) \rightarrow \text{MgF}_2(s)$

- Lattice energy -2913 kJ/mol
- I₁ of Mg 735 kJ/mol
- I₂ of Mg 1145 kJ/mol
- EA of F -328 kJ/mol
- Bond energy of F₂ 154 kJ/mol

- Sublimation of Mg 150 kJ/mol

3-5 Partial ionic character of covalent bonds

Three types of bonds:



Formula for percent ionic character of a bond

Defining ionic compounds

3-6 Covalent chemical bonds: A model

Models: An overview (text page 119)

- Models are human inventions based on incomplete understanding of nature
- Become more complicated as they mature
- Rely on underlying assumptions which limit the scope of conclusions we can make
- Wrong models teach us more than correct models

The covalent bond is a model

- Provides method for dividing up the energy released when a molecule is formed
- Bonding is a model for explaining molecular stability.
- e.g. CH₄ thought of not as 1 unit, but rather 4 x C-H units

3-7 Covalent bond energies and chemical reactions

Bond energy

Establishing the Sensitivity of Bonds to their Molecular Environment

Example: Stepwise decomposition of methane:



Types of bonds

- Single bond
- Double bond
- Triple bond



Bond energies

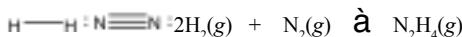
required.

released.

$$\Delta E = \sum n \times D(\text{bonds broken}) - \sum n > D(\text{bonds formed})$$

Example: Calculating ΔE for the reaction using bond energies.

Bond	Bond energy (kJ/mol)
------	-------------------------



3-8 The localized electron (LE) bonding model

- A molecule is composed of atoms bound together by sharing pairs of electrons using the valence atomic orbitals of the bound atoms
- Electrons are **localized** to one of the atoms or the space in between
 - Electron Pairs localized on specific atom: **lone pairs**

- Electron pairs localized to space between: **bonding pairs**

3 parts of the LE model:

1. Description of valence electron arrangement in the molecule using Lewis structures
2. Prediction of geometry of the molecule using the valence shell electron-pair repulsion (VSEPR) model
3. Description of type of atomic orbitals used by the atoms (for sharing or lone pairs)

3-9 Lewis Structures

Problem solving strategy: Writing Lewis Structures

- 1.
- 2.
- 3.
- 4.

Duet Rule:

Octet Rule:

Examples

Clicker (3.80)

Which of the following statements is true in describing the Lewis structure for H₂CO?

- A. There are three single bonds.
- B. Oxygen has three lone pairs of electrons around it.
- C. There is a double bond between carbon and oxygen.
- D. Carbon has a lone pair of electrons around it.
- E. There are two bonds between oxygen and hydrogen.

3-10 Exceptions to the octet rule

Examples

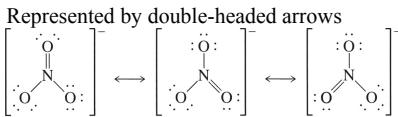
Review octet rule (text page 131)

- When writing the Lewis structure for a molecule, satisfy the octet rule for the atoms first. If electrons remain after the octet rule has been satisfied, then place them on any element from Period 3 or beyond.

3-11 Resonance

Condition where more than one valid Lewis structure can be written for a specific molecule

- Atoms need to be connected in the same order
- The resulting electron structure is derived from the average of the **resonance structures**



Formal charge

- Estimates the charge on all possible nonequivalent Lewis structures
- The difference between the number of valence electrons on the *free atom* and the number of electrons on the atom *in the molecule*

Equation:

Rules governing formal charge

- The sum of the formal charges of all atoms in a given molecule/ion must equal the overall charge
- If nonequivalent Lewis structures exist, those with formal charges closest to zero and with any negative formal charges on the most electronegative atoms are considered to best describe the bonding

Examples:

3-12 Naming simple compounds

Binary ionic compounds (Type I)

- Cation followed by an anion
- Cation is always named first and the anion second
- Monatomic cation: the name of the element
- Monatomic anion: root of the element name + ide

Binary ionic compounds (Type II)

- Some metals form more than one type of positive ion
 - Result: more than one type of ionic compound with a given anion
 - The charge on the metal ion is specified using Roman numerals.
 - Elements that form only one cation are not identified by Roman numerals.

Ionic compounds with polyatomic ions

Oxyanions: contain an atom plus oxygen atoms

- Series with two oxyanions:
 - Lesser number of oxygen atoms ends in *-ite*
 - Higher number of oxygen atoms ends in *-ate*
- Series with *more than* two oxyanions:
 - *Hypo-* prefix for the fewest oxygen atoms
 - *Per-* prefix for the most oxygen atoms

Binary covalent compounds (Type III)

Formed between two non-metals

Acids

- Molecules in which one or more H^+ ions are attached to an anion
- If the name of the anion ends in *-ide*, the acid is named with prefix *hydro-* and suffix *-ic*
 - The names of oxygen-containing anions are based on the root name of the anion, along with a suffix of *-ic* or *-ous*
 - If the name of the anion ends in *-ate*, the suffix *-ic* is added to the root name
 - If the name of the anion ends in *-ite*, the *-ite* is replaced by *-ous*