Part 2: Atomic Structure

2.2 Fundamental Chemical Laws

A. Law of Conservation of Mass (Lavoisier, 1789) –

B. Law of Definite Proportion (Proust, ~1800)

2.3 Dalton’s Atomic Theory (1808) –

A. Postulates of the theory:
B. Conclusions from Dalton’s Atomic Theory

- Which of these postulates is consistent with the Law of Conservation of Mass?

- Which of these postulates is consistent with the Law of Definite Proportions?

- Which of these postulates have since been modified?

2.4 Early Experiments to Characterize the Atom

A. The Electron – J.J. Thomson (1897)
2. Milikan’s Oil Drop Experiment (1909)

http://www.youtube.com/watch?v=O9Goyschazk
B. The Nuclear Atom

A. Parts of an Atom

Rutherford is credited with the "discovery" of the nuclear atom.

- Based on the alpha particle scatter pattern, Rutherford postulated in 1911 that the atom contains a very small, dense nucleus with the electrons surrounding the nucleus.
- Most of the volume of the atom is empty space.
- Protons were later "discovered" by Rutherford in 1919. (They were first detected by Eugen Goldstein in 1886, emitted in the opposite direction compared to electrons from a CRT.)
- Neutrons were finally discovered by James Chadwick in 1932.

**Model of the Atom**

- Electrons (–), e–
- Protons (+), p+
- Neutrons (0), n0
- Neutral atoms: number of protons = number of electrons

**Summary of Subatomic Particles**
Table 2.1: Summary of subatomic particles

<table>
<thead>
<tr>
<th>Particle</th>
<th>Grams</th>
<th>Relative Mass</th>
<th>Charge</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron</td>
<td>$9.109382 \times 10^{-28}$</td>
<td>0.0005485799</td>
<td>$-1$</td>
<td>$^0e$ or $e^-$</td>
</tr>
<tr>
<td>Proton</td>
<td>$1.672622 \times 10^{-24}$</td>
<td>1.007276</td>
<td>+1</td>
<td>$^1p$ or $p^+$</td>
</tr>
<tr>
<td>Neutron</td>
<td>$1.674927 \times 10^{-24}$</td>
<td>1.008665</td>
<td>0</td>
<td>$^0n$ or $n^0$</td>
</tr>
</tbody>
</table>

*These constants and others in the book are taken from the National Institute of Standards and Technology Web site at http://physics.nist.gov/cuu/Constants/index.html

B. Mass Spectrometry: The Discovery of Isotopes!
Table 2.2: Some Examples of Isotopic Abundances and Masses Determined Using Mass Spectrometry

<table>
<thead>
<tr>
<th>Element</th>
<th>Symbol</th>
<th>Atomic Weight</th>
<th>Mass Number</th>
<th>Isotopic Mass (amu)</th>
<th>Natural Abundance (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H</td>
<td>1.00794</td>
<td>1</td>
<td>1.0078</td>
<td>99.985</td>
</tr>
<tr>
<td></td>
<td>D⁺</td>
<td>2</td>
<td>2</td>
<td>2.0141</td>
<td>0.015</td>
</tr>
<tr>
<td></td>
<td>TⅠ</td>
<td>3</td>
<td>3</td>
<td>3.0161</td>
<td>0</td>
</tr>
<tr>
<td>Boron</td>
<td>B</td>
<td>10.811</td>
<td>10</td>
<td>10.0129</td>
<td>19.91</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>11</td>
<td>11.0093</td>
<td>80.09</td>
</tr>
<tr>
<td>Neon</td>
<td>Ne</td>
<td>20.1797</td>
<td>20</td>
<td>19.9924</td>
<td>90.48</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>21</td>
<td>20.9938</td>
<td>0.27</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>22</td>
<td>21.9914</td>
<td>9.25</td>
</tr>
<tr>
<td>Magnesium</td>
<td>Mg</td>
<td>24.305</td>
<td>24</td>
<td>23.9850</td>
<td>78.99</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>25</td>
<td>24.9858</td>
<td>10.00</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>26</td>
<td>25.9826</td>
<td>11.01</td>
</tr>
</tbody>
</table>

*D = deuterium; Ⅰ = tritium, radioactive

C. Atomic Number, Mass Number and Isotopic Notation

Lecture Examples:

a. How many electrons, protons and neutrons are contained in the isotope \( ^{35}_{17}Cl \)?

b. What is the isotopic notation for Uranium–235?
3.1 Counting by Weighing

3.2 Atomic Masses

A. Atomic mass unit (amu) -

Table 3.1: Subatomic particle masses in terms of atomic mass units:

<table>
<thead>
<tr>
<th>Particle</th>
<th>Mass(g)</th>
<th>Mass(amu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>proton</td>
<td>$1.6727 \times 10^{-24}$</td>
<td>1.007316</td>
</tr>
<tr>
<td>neutron</td>
<td>$1.6750 \times 10^{-24}$</td>
<td>1.008701</td>
</tr>
<tr>
<td>electron</td>
<td>$9.110 \times 10^{-28}$</td>
<td>0.0005486</td>
</tr>
</tbody>
</table>

Table 3.2: The mass of some atoms as determined by a mass spectrometer:

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Mass(amu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^2$H</td>
<td>2.0140</td>
</tr>
<tr>
<td>$^4$He</td>
<td>4.00260</td>
</tr>
<tr>
<td>$^8$Be</td>
<td>8.005305</td>
</tr>
<tr>
<td>$^{12}$C</td>
<td>12.000000</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>15.994915</td>
</tr>
<tr>
<td>$^{24}$Mg</td>
<td>23.985042</td>
</tr>
</tbody>
</table>
B. Masses of Isotopes

Lecture Example: The natural abundance of $^{63}\text{Cu}$ is 69.09\% and for $^{65}\text{Cu}$ is 30.19\%. If the atomic mass of $^{63}\text{Cu}$ is 62.93 amu and $^{65}\text{Cu}$ is 64.93 amu, what is the average atomic mass for natural copper?

3.3 The Mole

A. Defining the mole

Lecture example: Calculate the number of atoms contained in 5.0 mol and calculate the number of moles of electrons contained in $2.1 \times 10^{24}$ electrons.
Chapter 7: Quantum Theory

Before we get into quantum theory, let’s look at classical theory:

- Light behaves as a wave
- Electrons behave as particles
- Energy is continuous
- In the early 1900s observations were made that contradict classical theory.
- Quantum Theory explains the new observations.

7.1 Electromagnetic (EM) radiation –

A. Properties of a wave
Analogy: You are standing on a freeway overpass and there is one lane with constant stream of Mini Coopers and one lane with a constant stream of semi trucks (each travelling at the same speed). You count the # of Mini Coopers or semis that pass in a given amount of time.

Is the frequency of Mini Coopers or Semi Trucks larger?

Lecture Example: The light blue glow given off by Hg street lamps has a wavelength of 436 nm. What is its frequency?
B. The Electromagnetic (EM) Spectrum –

7.2 The Nature of Matter

A. Max Planck:
B. Photoelectric Effect Experiment (Einstein used Planck’s ideas to explain the photoelectric effect)
D. Summary of Planck and Einstein’s work
Lecture Examples

a. The wavelength of light is 594 nm. What is the energy of a photon of this light? Would light with a wavelength of 752 nm have a higher or lower energy per photon?

b. Calculate the frequency in megahertz and wavelength in meters of electromagnetic radiation with energy $6.527 \times 10^{-26}$ J/photon.

c. The light-sensitive substance in black-and-white photographic film is AgBr (back in the old days, film was needed for photos!). Photons provide the energy necessary to transfer an electron from Br$^-$ to Ag$^+$ to produce Ag and Br and thereby darken the film.
  i. If a minimum energy of $2.00 \times 10^5$ J/mol is needed for this process, what is the minimum energy needed by each photon?
ii. Calculate the wavelength of the light necessary to provide photons of this energy.

iii. Explain why this film can be handled in a darkroom under red light.

7.3 The Atomic Spectrum of Hydrogen

A. Emission Spectra -
B. H atoms in the gas phase exhibited the following spectrum:

![Graph of H atom spectrum]

7.4 The Bohr Model

A. Niels Bohr’s Description of the H-atom:
B. Energy of the electron

Lecture Example: Consider an electron in the H atom. What is the change in energy when the electron falls from n=6 to n=2? What wavelength light is emitted? What color is this light?
Lecture Example: What is the ionization energy for a ground state H atom and a mole of H atoms? In other words, how much energy does it take to remove an electron from the ground state of Hydrogen per atom and per mole of H atoms?

7.2 The Nature of Matter (revisited)

A. Matter has wave properties
Lecture Example: Calculate the wavelengths of the following matter:

a. a 145 g fastball moving at 95 miles per hour.

b. an electron moving at $1.0 \times 10^6$ m/s? The mass of an electron is $9.11 \times 10^{-31}$ kg.

“Think about it”-Why are we unable to observe wave-like motions for macroscopic objects such as baseballs and people?

7.5 The Quantum Mechanical Model of the Atom –

A. Heisenberg Uncertainty Principle –
B. The Birth of Quantum Mechanics: the Schrödinger Equation

The Nobel Prize in Physics in 1933 was awarded jointly to Erwin Schrödinger and Paul Adrien Maurice Dirac “for the discovery of new productive forms of atomic theory”
7.6 Quantum Numbers – Obtained from the results of solving the Schrodinger equation

A. Intro to Quantum Numbers

B. Principle Quantum Number (n)
C. Angular Momentum Quantum Number (l)

D. Magnetic Quantum Number (m_l)
E. Allowed Orbitals and Quantum Numbers

Table 7.1 – Relationship Between $n$, $l$, and $m_l$ through $n = 4$

<table>
<thead>
<tr>
<th>$n$</th>
<th>Possible values of $l$</th>
<th>Subshell Designation*</th>
<th>Possible values of $m_l$</th>
<th>Number of Orbitals in Subshell</th>
<th>Total Number of Orbitals in Shell</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.7 Orbital Shapes and Energies

A. Each value of $l$ describes a different orbital shape.
B. The s orbital shape

C. The p orbital shapes

D. The d orbital shapes

E. Radial Electron Density Functions — s Orbitals
7.8 Electron Spin and the Pauli Principle

A. Electron spin quantum number \( m_s \)
B. The Pauli Exclusion Principle

Table 7.2: Orbitals and the maximum number of electrons

<table>
<thead>
<tr>
<th>Subshell</th>
<th># of orbitals</th>
<th>Maximum # of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>s</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p</td>
<td></td>
<td></td>
</tr>
<tr>
<td>d</td>
<td></td>
<td></td>
</tr>
<tr>
<td>f</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.9 Polyelectronic Atoms

A. H atom

B. All other atoms – polyelectronic atoms
Hydrogen Energy Levels

Multi-electron Energy Levels

Electrons outside have no effect on effective nuclear charge for electron of interest.

Positively charged nucleus.

Electrons between electron of interest and nucleus cancels some of the positive nuclear charge.

Inner electrons

Attraction

Repulsion

Outer electron

Nucleus

3s Shields 3p

Electrons in 3p have higher energy
7.11 The Aufbau Principle and the Periodic Table

A. Aufbau Principle

B. Electron Configurations (most probable address of electron)

<table>
<thead>
<tr>
<th>1. Regular Notation</th>
<th>2. Orbital Diagram</th>
<th>3. Noble Gas (Condensed) Configuration</th>
</tr>
</thead>
</table>
C. Hund’s Rule

D. Terms Relating to Electrons

Lecture Example: Write the electron configuration, the condensed electron configuration, determine if the following are paramagnetic or diamagnetic and list the number of valence electrons

a. $O$

b. $S$

c. $Ne$

d. $Ar$
7.12 Periodic Trends in Atomic Properties

**A. Atomic Radii**

<table>
<thead>
<tr>
<th></th>
<th>Incr/Decr?</th>
<th>Why?</th>
</tr>
</thead>
<tbody>
<tr>
<td>↓ a group</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
B. Electron Affinity –

<table>
<thead>
<tr>
<th>→ a period</th>
<th></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>↓ a group</th>
<th></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>→ a period</th>
<th></th>
</tr>
</thead>
</table>
### C. Ionization Energy –

<table>
<thead>
<tr>
<th></th>
<th>Incr/Decr?</th>
<th>Why?</th>
</tr>
</thead>
<tbody>
<tr>
<td>↓ a group</td>
<td></td>
<td></td>
</tr>
<tr>
<td>→ a period</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

7.13/8.4 Metals and Nonmetals – Electron Configurations and More

A. Metals

1. Metals in Groups 1A and 2A -
2. Metals in Groups 3A and 4A and Transition Metals

B. Nonmetals

C. Metalloids