University Chemistry I

Chemistry 120, Section A

Chapter 7 — Atomic Structure and Periodicity

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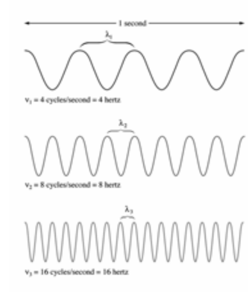
7-1

Electromagnetic Radiation — Waves

Fig. 7.1 Zumdahl and Zumdahl, 6th Ed.

Radiant energy that exhibits wavelength-like behavior and travels through space at the speed of light in a vacuum.

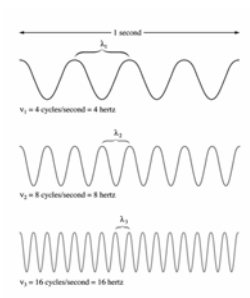


7-2

Waves Have Three Primary Characteristics

Fig. 7.1 Zumdahl and Zumdahl, 6th Ed.

1. Wavelength (λ): distance between two peaks (or troughs) in a wave.
2. Frequency (ν): number of waves per second that pass a given point in space.
3. Speed (c): speed of light is 2.9979×10^8 m/s.



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Wavelength and Frequency Can Be Interconverted

$$\lambda\nu = c \quad \text{or} \quad \nu = \frac{c}{\lambda}$$

ν = frequency (s^{-1}, AKA Hz)

λ = wavelength (m)

c = speed of light ($m\ s^{-1}$)

Short wavelength, high energy

7-4

Sample Problem

- What is the frequency of light with a wavelength of 340 nm?

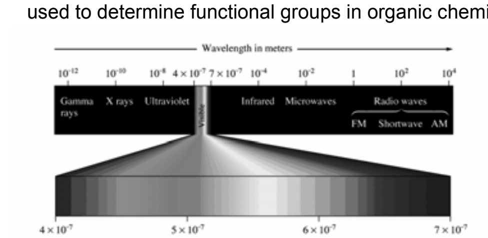
$8.8 \times 10^{14}\ sec^{-1}$

7-5

Electromagnetic Radiation — Spectrum

Fig. 7.2 Zumdahl and Zumdahl, 6th Ed.

Visible light is a small portion of the spectrum, and other regions can be used to study atomic and molecular structure. For example, infrared (IR) spectroscopy is used to determine functional groups in organic chemistry.

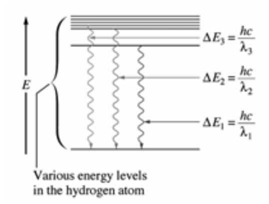


7-6

Using Light to Study Atoms

Fig. 7.7 Zumdahl and Zumdahl, 6th Ed.

- Electrons can be stimulated from a *ground state* to an *excited state* by giving them energy.
- If electrons go back to the ground state, they must release energy.
- The energy is released as light.

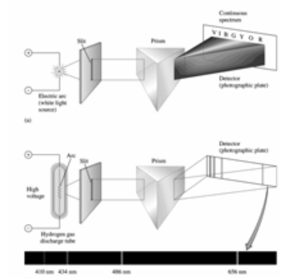


7-7

Atomic Spectrum of Hydrogen

Fig. 7.6b Zumdahl and Zumdahl, 6th Ed.

- A continuous spectrum contains all the wavelengths of light (white light).
- A line spectrum (AKA discrete spectrum) contains only some of the wavelengths of light.
- The hydrogen atom displays a line spectrum, demonstrating that energy is *quantized*.



7-8

Planck's Constant

Transfer of energy is quantized, and can only occur in discrete units, called quanta.

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

ΔE = change in energy, in J

h = Planck's constant, 6.626×10^{-34} J s

ν = frequency, in s^{-1}

λ = wavelength, in m

This means that matter is not continuous

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Sample Problem

- What is the "packet size" of light with a wavelength of 340 nm?

5.8×10^{-19} J

7-10

Energy and Mass

- Energy has mass

$$E = mc^2$$

where *E* = energy

m = mass

c = speed of light

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Energy and Mass

$$E_{\text{photon}} = \frac{hc}{\lambda}$$

$$m_{\text{photon}} = \frac{h}{\lambda c}$$

(Hence the dual nature of light.)

7-12

X-ray Diffraction

Fig. 7.5 Zumdahl and Zumdahl, 6th Ed.

Relationship to Wavelength and Mass

de Broglie's Equation

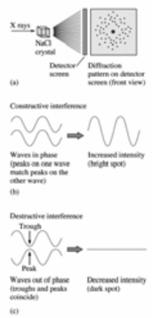
$$\lambda = \frac{h}{m\nu}$$

λ = wavelength, in m

h = Planck's constant, 6.626×10^{-34} J s = kg m^2 s^{-1}

m = mass, in kg

ν = frequency, in s^{-1}



7-13

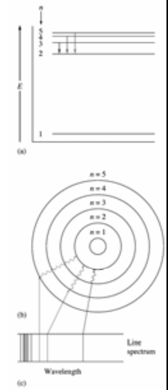
The Bohr model of the Hydrogen Atom

Fig. 7.8 Zumdahl and Zumdahl, 6th Ed.

- Bohr model: The electron in a hydrogen atom moves around the nucleus only in certain allowed circular orbits.

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

- where n = integer
  Z = nuclear charge



7-14

Sample Test Question and Point

- How much energy is required to move the electron of hydrogen from its ground state (n=1) to its third excited state (n=?)?
- Page 297: "... *all matter exhibits both particulate and wave properties*. Large pieces of matter, such as baseballs, exhibit predominately particulate properties....Very small "bits of matter", ...exhibit predominately wave properties."

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Good News and Bad News

- Bohr's model predicts very well the electron distribution of hydrogen (Z=1).
- The model doesn't work for Z=2 or any other number.

7-16

The Bohr Model

Ground State: The lowest possible energy state for an atom (n = 1).

Excited States: Any energy level other than the lowest possible, n = 2, 3, 4…

7-17

Energy Changes in the Hydrogen Atom

$$\Delta E = E_{\text{final state}} - E_{\text{initial state}}$$

7-18

Quantum Mechanics

- Based on the wave properties of the atom
  $\hat{H}\Psi = E\Psi$
- Ψ = wave function
- $\hat{H}$ = mathematical operator
- E = total energy of the atom
- A specific wave function is often called an orbital.

7-19

Heisenberg Uncertainty Principle

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

- *x* = position
- *mv* = momentum
- *h* = Planck's constant

The more accurately we know a particle's position, the less accurately we can know its momentum.

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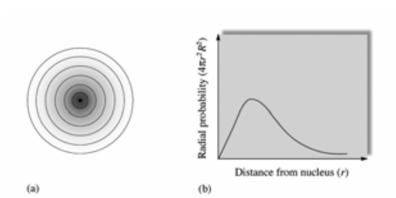
Probability Distribution

Fig. 7.12 Zumdahl and Zumdahl, 6th Ed.

- square of the wave function
- probability of finding an electron at a given position
- Radial probability distribution is the probability distribution in each spherical shell.



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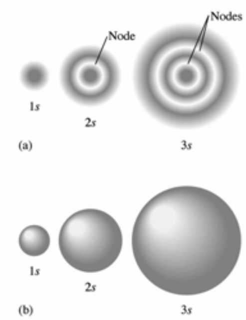
Quantum Numbers (QN) — Principal QN

Fig. 7.13 Zumdahl and Zumdahl, 6th Ed.

1. Principal QN (*n* = 1, 2, 3, . . .) - related to size and energy of the orbital.



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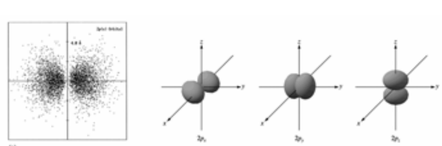
Quantum Numbers — Angular Momentum

Fig. 7.14 Zumdahl and Zumdahl, 6th Ed.

1. Principal QN (*n* = 1, 2, 3, . . .) - related to size and energy of the orbital.
2. Angular Momentum QN (*l* = 0 to *n* − 1) - relates to shape of the orbital.

l=0, s; *l*=1, p; *l*=2, d; *l*=3, f



7-23

Quantum Numbers — Angular Momentum

Fig. 7.14 Zumdahl and Zumdahl, 6th Ed.

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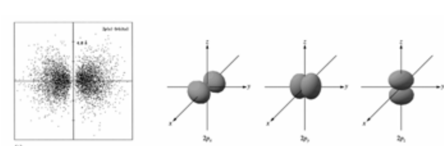
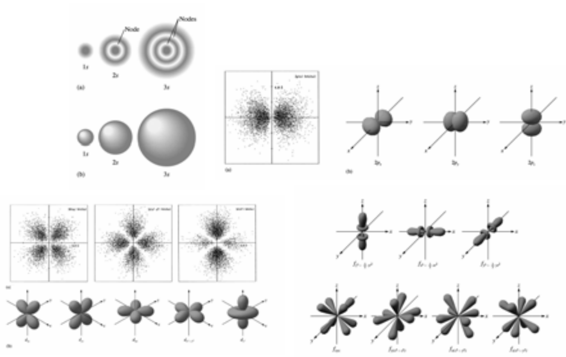
2. Angular Momentum QN (*l* = 0 to *n* − 1) - relates to shape of the orbital.
3. Magnetic QN (m_l = l to −l) - relates to orientation of the orbital in space relative to other orbitals.



7-24

Shapes and Orientations of Orbitals

Figs. 7.13, 7.14, 7.16 and 7.17 Zumdahl and Zumdahl, 6th Ed.



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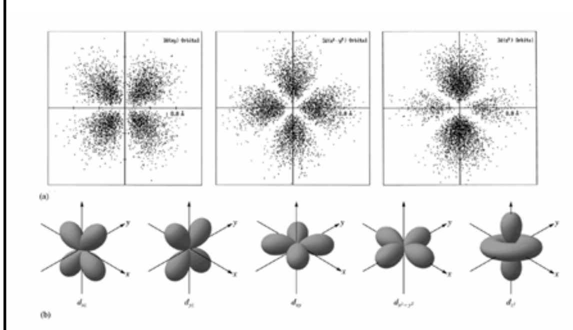
Shapes and Orientations of Orbitals

Fig. 7.16 Zumdahl and Zumdahl, 6th Ed.



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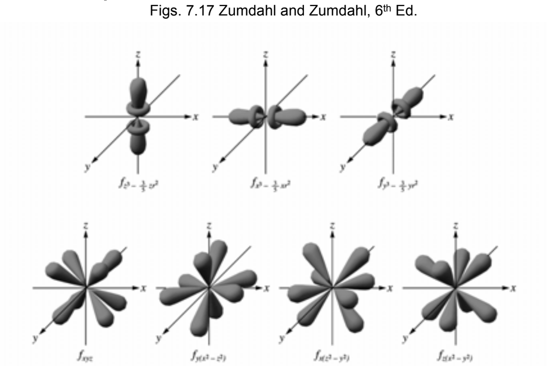
Shapes and Orientations of Orbitals

Figs. 7.17 Zumdahl and Zumdahl, 6th Ed.



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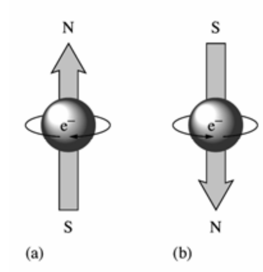
Quantum Numbers (QN) — Principal QN

Fig. 7.19 Zumdahl and Zumdahl, 6th Ed.

1. Principal QN (n = 1, 2, 3, . . .) - related to size and energy of the orbital.
2. Angular Momentum QN (l = 0 to n – 1) - relates to shape of the orbital.
3. Magnetic QN (m_l = l to –l) - relates to orientation of the orbital in space relative to other orbitals.
4. Electron Spin QN (m_s = +1/2, –1/2) - relates to the spin states of the electrons.



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Pauli Exclusion Principle

- In a given atom, no two electrons can have the same set of four quantum numbers (n, l, m_l, m_s).
- *Therefore*, an orbital can hold only two electrons, and they must have opposite spins.

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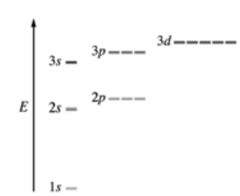
Putting Things Together

Table 7.2, Fig. 7.22 Zumdahl and Zumdahl, 6th Ed.

TABLE 7.2 Quantum Numbers for the First Four Levels of Orbitals in the Hydrogen Atom

n	ℓ	Orbital Designation	m_ℓ	Number of Orbitals
1	0	1s	0	1
2	0	2s	0	1
	1	2p	−1, 0, +1	3
3	0	3s	0	1
	1	3p	−1, 0, 1	3
	2	3d	−2, −1, 0, 1, 2	5
4	0	4s	0	1
	1	4p	−1, 0, 1	3
	2	4d	−2, −1, 0, 1, 2	5
	3	4f	−3, −2, −1, 0, 1, 2, 3	7



7-30

Aufbau Principle

- German for “building up”
- As protons are added one by one to the nucleus to build up the elements, electrons are similarly added to these hydrogen-like orbitals.

7-31

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.

Another way of putting this is that electrons spread out so they have ‘elbow room’

Referred to as “degenerate”

7-32

Electron Configuration Notations

- Go through 1st 10 elements

Review

- 52a. Calculate the wavelength of light emitted when each of the following transitions occur in the hydrogen atom. What type of EM radiation is emitted in each transition?
- N=4 to n=3
- 42. a photon of UV light possesses enough energy to mutate a strand of human DNA. What is the E of a single UV photon having a wavelength of 25 nm?

7-33

Valence Electrons

The electrons in the outermost principle quantum level of an atom.

Inner electrons are called core electrons.

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Broad Periodic Table Classifications

- Metals and nonmetals previously pointed out
- Main Group Elements (representative): filling s and p orbitals (Na, Al, Ne, O)
- Transition Elements: filling d orbitals (Fe, Co, Ni)
- Lanthanide and Actinide Series (inner transition elements): filling 4f and 5f orbitals (Eu, Am, Es)

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Electron Configuration of Transition and Inner Transition Elements There are Some Surprises!

- Uranium:
  $1s^2 2s^2 p^6 3s^2 p^6 d^{10} 4s^2 p^6 d^{10} f^{18} 5s^2 p^6 d^{10} f^3 6s^2 p^6 d^1 7s^2$
  $\rightarrow$ [Rn]$5f^3 6d^1 7s^2$ much simpler
- Nickel [Ar]$3d^8 4s^2$
- Copper [Ar]$3d^{10} 4s^1$

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Periodic Trends: Ionization Energy

Ionization Energy- The quantity of energy required to remove an electron from the gaseous atom or ion.

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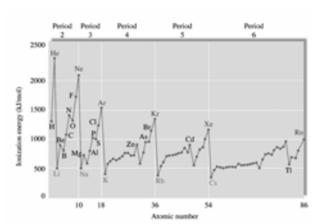
Periodic Trends: Ionization Energy

Fig. 7.31 Zumdahl and Zumdahl, 6th Ed.

First ionization energy- the amount of energy required to take the first electron away from an atom.

Periodic trend: increases $\rightarrow$ across a period, going $\uparrow$ a group.

He is the element with the largest ionization energy.



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Periodic Trends: Electron Affinity

The energy change associated with the addition of an electron to a gaseous atom.

- $X(g) + e^- \rightarrow X^-(g)$

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Periodic Trends: Electronegativity

Electronegativity- how strongly an atom pulls on another atoms electrons.

Periodic trend: increases $\rightarrow$ across a period, going $\uparrow$ a group.

But, **F** is the element with the largest electronegativity, not He.

Chart I. Electronegativities of Selected Elements

H 2.21								He —
Li 0.98	Be 1.57		B 2.04	C 2.55	N 3	O 3.44	F 3.98	Ne —
Na 0.93	Mg 1.31		Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar —
K 0.82	Ca 1.00		Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr —
Rb 0.82	Sr 0.95		In 1.78	Sn 1.96	Sb 2.05	Te 2.10	I 2.66	Xe —
Cs 0.79	Ba 0.89		Tl 2.04	Pb 2.33	Bi 2.02	Po 2.0	At 2.2	Rn —

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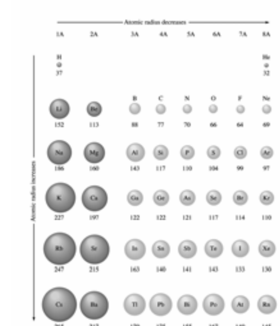
Periodic Trends: Size

Fig. 7.35 Zumdahl and Zumdahl, 6th Ed.

Atomic Radii (Size)-

Periodic trend: increases $\leftarrow$ across a period, going $\downarrow$ a group.

Cs is the largest (known) atom



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Periodic Trends: mp/bp

melting point- temperature at which something goes from a solid to a liquid.

boiling point- temperature at which something goes from a liquid to a gas.

Periodic trend: increases → ← across a period, going ↓ a group.

W is the element with the highest mp, 3680 K; and bp, 5828 K.

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Information Contained in the Periodic Table

1. Each group member has the same valence electron configuration (these electrons primarily determine an atom's chemistry).
2. The electron configuration of any main group element.
3. Certain groups have special names (alkali metals, halogens, etc).

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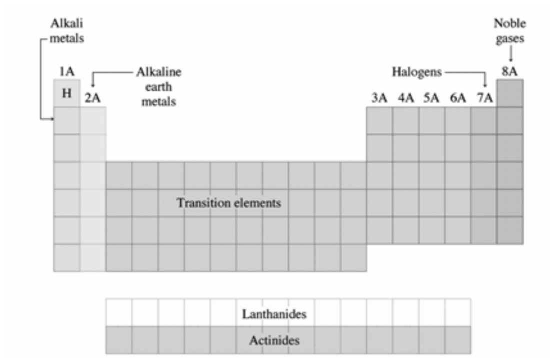
Certain Groups Have Special Names



7-44

Information Contained in the Periodic Table

1. Each group member has the same valencec electron configuration (these electrons primarily determine an atom's chemistry).
2. The electron configuration of any main group element.
3. Certain groups have special names (alkali metals, halogens, etc).
4. Metals and nonmetals are characterized by their chemical and physical properties.

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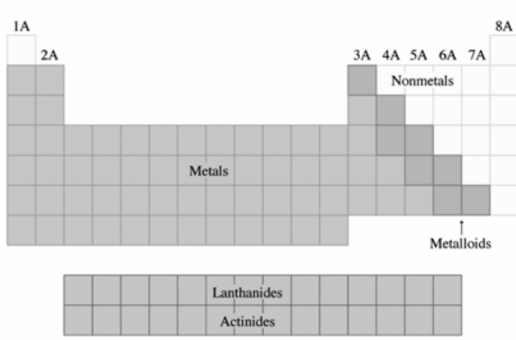
Metals, Nonmetals and Metalloids



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Properties of Metals and Nonmetals

Metal	*Metalloid*	Nonmetal
solid	*intermediate properties*	liquid or gas
shiny		dull
malleable/ductile		brittle
conductive	*semiconductors*	insulators
like to give up e^-		like to take up e^-