Atomic and Electronic Structure (Chapter 7)

(Quantum-Mechanical Model of the Atom)

Electromagnetic Radiation and Atomic Spectra

1. Electromagnetic Radiation -- Light

   wavelength: λ

   frequency: ν

   $\lambda\nu = c$ = speed of light = 3.00×10^{8} m/sec

   units: λ = distance (m, cm, nm, etc.)
   ν = 1/sec = s^{-1} { 1 s^{-1} = 1 Hertz }

   electromagnetic spectrum -- range of frequencies / wavelengths (see **Figure 7.5**)

2. Energy of electromagnetic radiation

   Radiation interacts with matter in discrete "packets" of energy called "quanta" or "photons".

   $E = h\nu$ where h = Planck's Constant = 6.63×10^{-34} J·sec

   Atomic Spectra:

   Energetically excited atoms only emit radiation in discrete energies corresponding to the atom's electronic energy levels.

3. Atomic Spectra

   Energetically excited atoms only emit radiation in discrete energies corresponding to the atom's electronic energy levels. (see **Figure 7.11**)

4. Bohr model of H atom

Energy levels: $E = -b / n^2$

where n is a "quantum number" with possible values of:

n = 1, 2, 3, 4,..... (see **Figure 7.12**)

{increasing value of n indicates an electron "orbit" farther from the nucleus}

It is possible to calculate energy differences between levels (i.e., the atomic spectrum) with different n values -- see textbook

Electronic Quantum Numbers

Electrons in multi-electron atoms are arranged

in a series of **shells ⟶ subshells ⟶ orbitals**

file cabinet analogy: drawers ⟶ file folders ⟶ papers

Each orbital can be described mathematically by a "wave function" that is characterized by a set of ***quantum numbers***.

1. Principle Quantum number -- n

related to **energy** of ***shell*** and to distance from nucleus (size)

possible values of **n = 1, 2, 3, 4**, ...

2. Secondary Quantum Number -- l

related to **shape** of various ***subshells*** within a given ***shell***

possible values of **l = 0 1 2 3 4 ..... n - 1**

letter designation: **s p d f g .....**

values of n	values of l	subshells
1	0	1s
2	0, 1	2s, 2p
3	0, 1, 2	3s, 3p, 3d

3. Magnetic Quantum Number -- m_l

related to **spatial orientation** of ***orbitals*** within a given ***subshell***

possible values of **m_l = - l, ... 0, ..., + l**

the number of m_l values = number of orbitals within a subshell

e.g., within a subshell having l = 2, there are 5 orbitals corresponding to the 5 possible values of m_l (- 2, -1, 0, +1, +2)

Summary -- electronic quantum numbers and orbitals

n	l	m_l	subshell	# orbitals
1	0	0	1s	1
2	0	0	2s	1
	1	-1. 0, +1	2p	3
3	0	0	3s	1
	1	-1, 0, +1	3p	3
	2	-2, -1, 0, +1, +2	3d	5
4	0	0	4s	1
	1	-1, 0, +1	4p	3
	2	-2, -1, 0, +1, +2	4d	5
	3	-3, -2, -1, 0, +1, +2, +3	4f	7

4. Electron Spin and the Pauli Exclusion Principle

electrons have intrinsic angular momentum -- **"spin"** -- **m_s**

possible values: **m_s = +1/2 and -1/2** (only two possible values)

Pauli Exclusion Principle:

No two electrons in an atom can have identical values of all 4 quantum numbers -- maximum of 2 electrons per orbital!

a single orbital can hold a "pair" of electrons with opposite "spins"

e.g., the 3rd shell (n = 3) can hold a maximum of 18 electrons:

n = 3	l =	0	1	2	
	subshell	3s	3p	3d	
	# orbitals	1	3	5	
	# electrons	2	6	10 =	18 total

A single electron in an orbital is called "unpaired." Atoms with 1 or more unpaired electrons are ***paramagnetic***, otherwise they are ***diamagnetic***

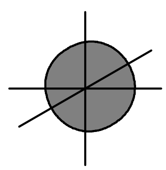
Shapes of Atomic Orbitals

Atomic orbitals are best viewed as "clouds of electron density" and represented as contour plots of the probability of finding the electron.

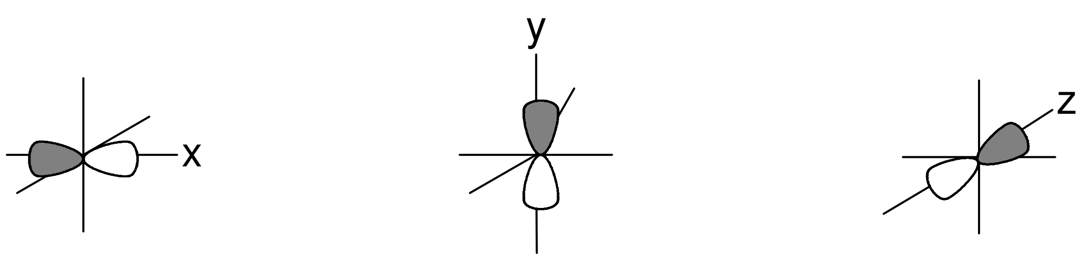
nodal surface an imaginary point, plane, or spherical surface where the probability of finding the electron is equal to zero

simplified pictures

s orbitals are spherical shaped



p orbitals are "bow tie" shaped and **oriented** along the coordinate axes



P_x P_y P_z

d orbitals have more complex shapes (see text)