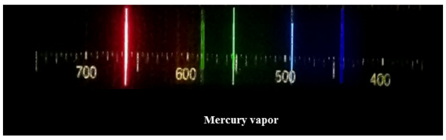
7.3 - 7.9 - Atomic Spectra and Quantum Numbers

Atomic Emission Spectra (AES)

Heated elements emit a spectrum, allowing every element to be identified (like a fingerprint).

This is not a continuous spectrum, like white light, but banded at particular frequencies. (Demo: Fluorescent Lights)



Quantum Theory & the Atom

Niels Bohr (1913) proposed a model to explain AES:

Electrons reside only in specific levels (circular orbits) in an atom, like unevenly spaced rungs of a ladder.

They absorb (and emit) specific amounts of energy during moves between levels.

Electrons start at a ground state, and become excited from this level by absorbing energy.

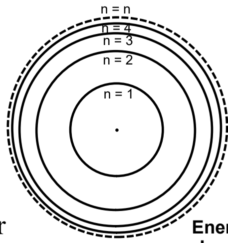
Niels Bohr

Atomic Energy Levels

Electrons can be thought of as moving on rungs of a ladder (principal quantum numbers: **n**): when they gain energy they move up; when they lose energy they move down.

The lowest level is the ground state (n = 1), and they become excited by adding energy.

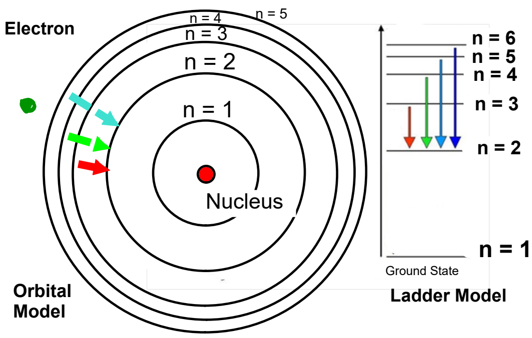
Electrons jump between levels willy-nilly, absorbing or emitting photons as they do.



Energy Level Model

Hydrogen Spectrum Demo

Observe the spectrum of hydrogen. The discreet colors seen correspond to the following transitions:



Mathematics of the Bohr Model

Bohr derived an equation that governed the energy transition for hydrogen's electron jumping from one level to another:

$$E = -2.178E-18J\left(\frac{1}{n_{final}^{2}} - \frac{1}{n_{initial}^{2}}\right)$$

n = integer value (energy levels)

Energy perspectives must be addressed: the electron is considered to lose energy as it approaches the nucleus.

In order to reach energy levels farther away, it must gain energy.

Electron Energies

1. Calculate the energy required to excite the hydrogen electron from $n = 1$ to $n = 2$.

2. What wavelength is this?

3. Calculate the energy required to completely remove hydrogen's electron from its ground state.

Electron Energies Answer (Slide 1)

1. Energy from $n = 1$ to $n = 2$.

$$E = -2.178E-18J\left(\frac{1}{n_{final}^{2}} - \frac{1}{n_{initial}^{2}}\right)$$

$$= -2.178E-18J\left(\frac{1}{2^2} - \frac{1}{1^2}\right) = \boxed{1.634E-18J}$$

Note: a positive amount of energy shows that the electron absorbs this energy to transition.

2. Wavelength:

Planck's Equation:

$$E = h\nu$$

$$\nu = \frac{E}{h} = \frac{1.634E-18J}{6.63E-18J{\bullet}s} = 2.465E15Hz$$

Finally:

$$\lambda = \frac{c}{\nu} = \frac{3.00E8m/s}{2.465E15Hz} = \boxed{1.22E-7m}$$

Electron Energies Answer (Slide 2)

3. Energy required to remove hydrogen's electron from the ground state.

Consider that the final level is some n which could be considered infinity for calculational purposes:

$$E = -2.178E-18J\left(\frac{1}{n_{final}^{2}} - \frac{1}{n_{initial}^{2}}\right)$$

$$= -2.178E-18J\left(\frac{1}{\infty} - \frac{1}{1^2}\right) = \boxed{2.178E-18J}$$

Limits to the Bohr Model

Bohr's model only explains hydrogen, not any other element's observed spectrum.

His model also doesn't account for the chemical behavior of atoms.

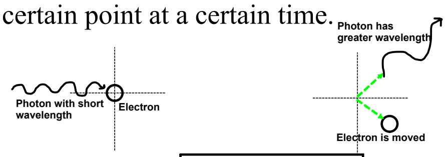
By the mid 1920's, it was abundantly evident that another model was necessary.

Heisenberg Uncertainty Principle

How do you find a floating balloon in a dark room?

Werner Heisenberg postulated: it is impossible to take any measurement of an object without disturbing it.

The upshot: you can't determine the path of an electron in orbit, only a probability that it will be at a certain point at a certain time.



Werner Heisenberg

Mathematically $\boxed{\Delta x \bullet \Delta(mv) \geq \frac{h}{4\pi}}$

Δx = uncertainty in a particle's location,
$\Delta(mv)$ = uncertainty in a particle's momentum,
h = Planck's constant.

Wave Equation

In 1926 Erwin Schrodinger devised an equation that worked for all elements.

His model treats electrons as waves, assigning a probability that they will be found somewhere around a nucleus.

Erwin Schrodinger

This model unlocked the different shapes of electron's energy levels.

His wave equation: $\hat{H}\psi = E\psi$ is a function of the x, y, and z coordinates of the electron's position in three-dimensional space and H is a set of mathematical instructions called an *operator*.
The symbol ψ is called "the wave function".
E represents the total energy of the atom.

Quantum Numbers

The wave equation requires that several components are needed to describe where an electron will be:

Principal quantum number (n): integral values relating to the size and energy of the orbital. As n increases, the electron ranges farther from the nucleus. In the periodic table, the number of elements requires 7 energy levels at ground state.

Angular momentum quantum number (l): integral values from 0 to n - 1 for each value of n. This relates to the shape of the subshell (sublevel), **commonly denoted s, p, d, and f** (beyond these: g, h, i, . . .).

Quantum Numbers

Magnetic quantum number (m_l): integral values between l and -l, including zero.
This value is related to the orientation of the orbital in space relative to the other orbitals. S has 1, p has 3, d has 5, and f has 7 orbitals.

Electron Spin quantum number (m_s): a fourth number was necessary to account for details of the emission spectra of atoms. In an external magnetic field, electrons were observed to have two possible magnetic moments, so electrons are assigned either an 'up' spin, or 'down' spin (based on the observed phenomenon that a rotating charge produces a magnetic field).

Subshells Example

4. For the principle quantum level n = 5, determine the allowed number of subshells (different values of l), and give the designation of each.

For n = 5, l values go from 0 to 4 (l = n - 1 in integer increments):

l = 0: 5s l = 1: 5p l = 2: 5d l = 3: 5f l = 4: 5g

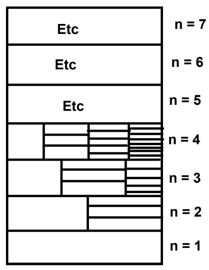
Orbital Structure Summary

Ground-state electrons of all 118 possible (at this time) elements occupy up to 7 energy levels (n).
Ex: Really odd 7 story apartment building.

Levels have sublevels (l):
s, p, d, f according to shape.
1st level has one, 2nd has two, etc.
Ex: apartments per floor.

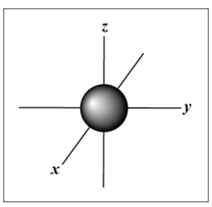
Sublevels have orbitals (m_l):
s = 1 p = 3 d = 5 f = 7
Ex: rooms per apartment

Each orbital holds two electrons with opposite spin (m_s).
Ex: two people per room.



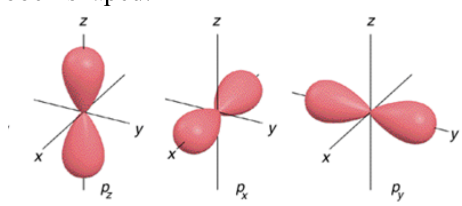
S Sublevel = 1 Orbital

Spherical:



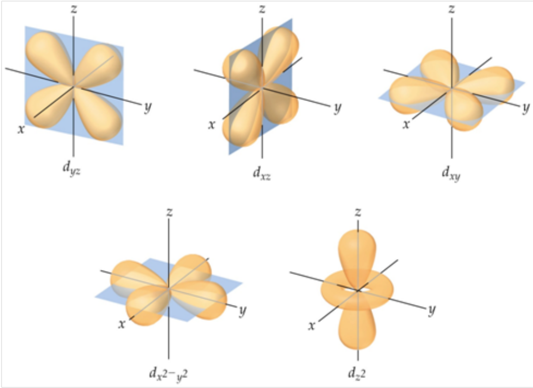
P Sublevel = 3 Orbitals

Dumbbell shaped:



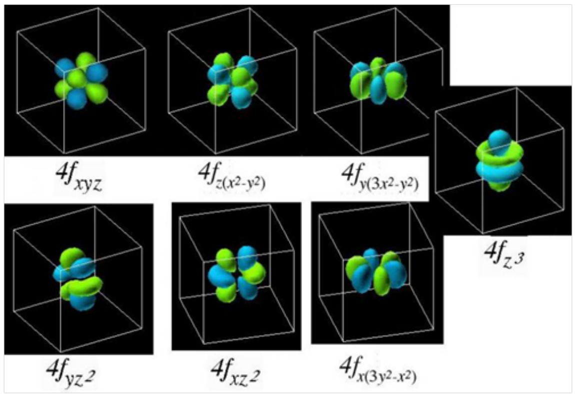
D Sublevel = 5 Orbitals

Double Dumbbell shaped:



F Sublevel = 7 Orbitals

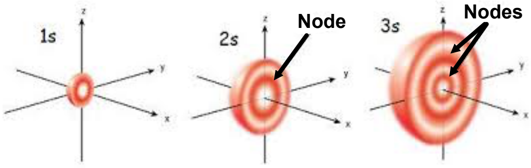
Bizarrely shaped:



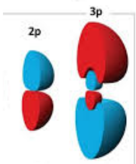
Sublevel Profiles

The probability cloud of sublevels with different *n* values becomes more complex at higher levels.

In comparing the 1s, 2s and 3s sublevels, nodes of low probability form.



Comparing 2p and 3p sublevels:



Homework

Preview 12.3

12.1-.2 Problems in your Booklet
Due: Next Class