# Chapter 7 Quantum Theory and Electronic Structure of Atoms (Ch7 Chang, Ch7 Jespersen)

The Wave Nature of Light

Electromagnetic *radiation* (defined on next slide) can be described as light energy and/or a wave.

A wave is a *vibrating disturbance* by which *energy* is *transmitted*.

Waves are characterized by their length, height and by the number of waves that pass a certain point in one second.
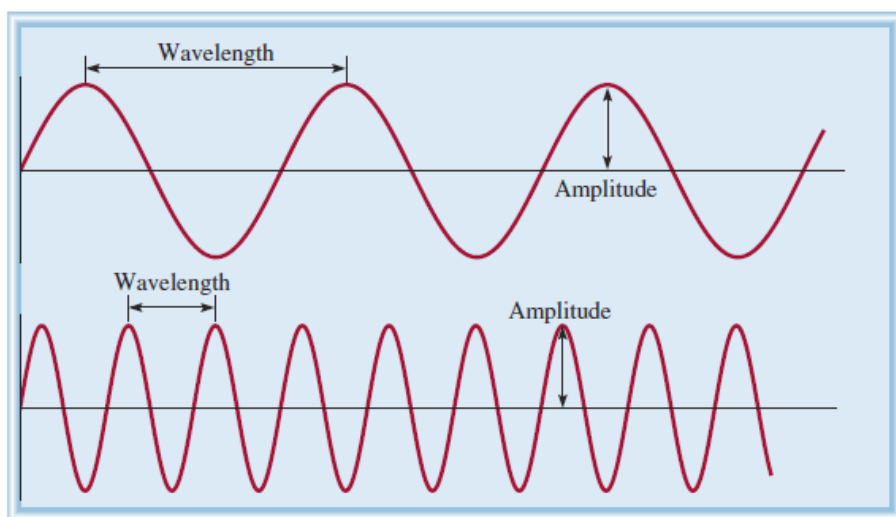
Wavelength, λ, in meters or nanometers.

Frequency, ν, in $\frac{1}{s}$ or s^{-1}, also Hz.

These two waves have the same amplitude; but the top wave has longer *wavelength*, and the lower wave has higher *frequency*.

Wavelength is the distance between *identical* points on *successive* waves.

Frequency is the number of waves that *pass* a *point* in *one second*.

Amplitude is the vertical distance from the *midline* of the wave to the *peak* (or *trough*).

The speed of a wave is also important, and depends on the *type* of wave, and the *medium* of travel.

Speed of a wave = **wavelength** x **frequency**

$$= \lambda \nu$$

UNIT CHECK $\qquad m \cdot s^{-1} \qquad = \qquad m \ s^{-1}$

There are many *types* of waves; here we are concerned with waves that have systematic fluctuations in intensities of electrical and magnetic components, which Maxwell in 1873 called Electromagnetic waves, of which *light* is an example.

The *transmission* (and emission) of *energy* in the form of *electromagnetic* waves is called Electromagnetic radiation.

The speed of electromagnetic waves (e.g. light), is a constant in a given medium.

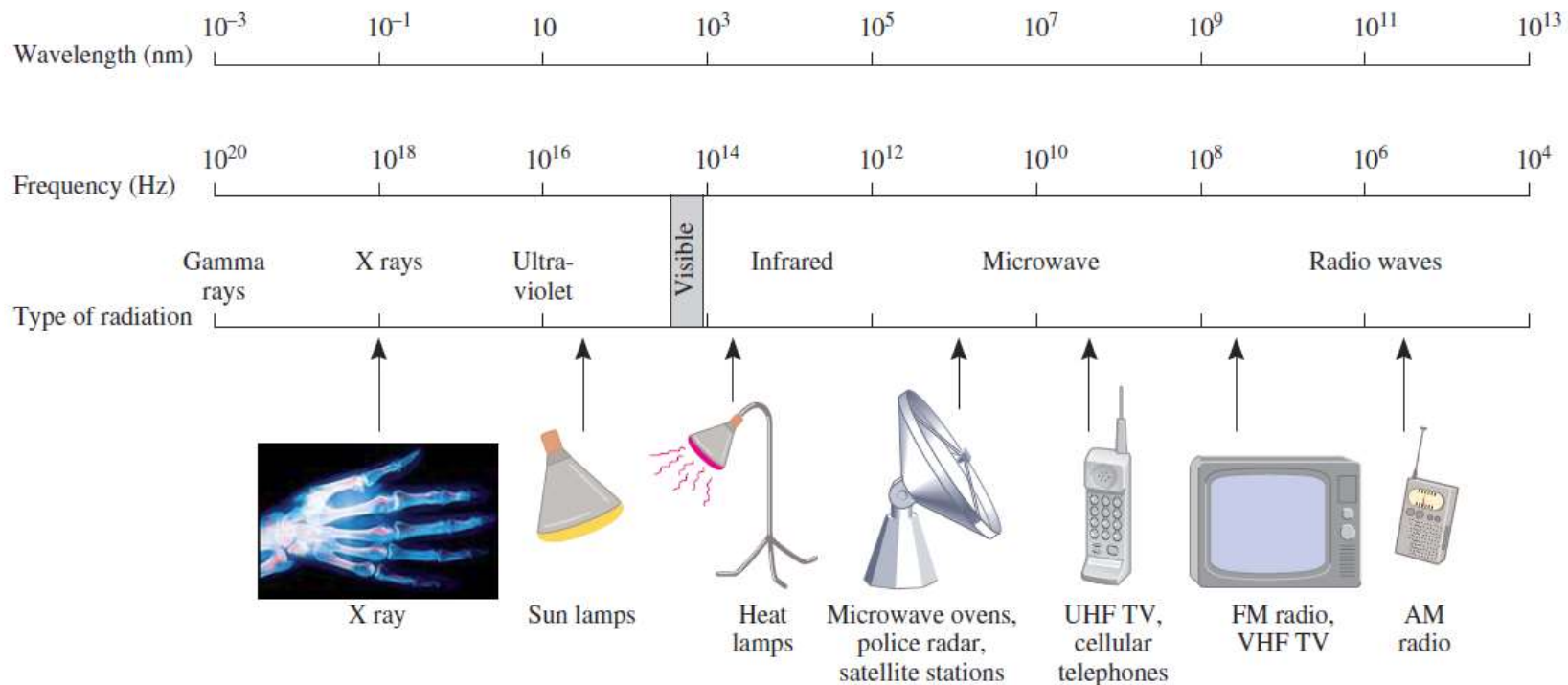The speed of light, c, is approx. **3.00 x 10^8 m/s** in a *vacuum*.

Often use the eqn: $c = \lambda \nu$

The *wavelength* of electromagnetic radiation is often reported in nanometers (nm) which is 10^{-9} m.

Electric field component

Magnetic field component
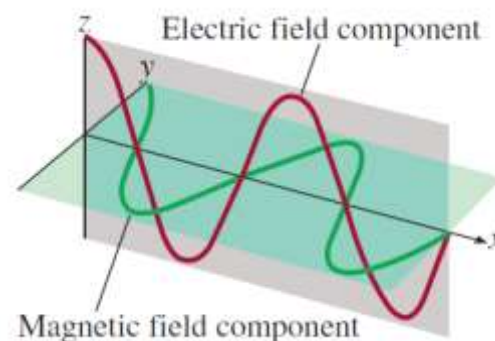
The Electromagnetic Spectrum

NOTICE: Energy increases ⇐   Wavelength increases ⇒   Frequency increases ⇐

Wavelength (nm)	10^{-3}	10^{-1}	10	10^3	10^5	10^7	10^9	10^{11}	10^{13}

Frequency (Hz)	10^{20}	10^{18}	10^{16}	10^{14}	10^{12}	10^{10}	10^8	10^6	10^4

Type of radiation   Gamma   X rays   Ultra-   Visible   Infrared   Microwave   Radio waves
rays   violet

X ray   Sun lamps   Heat   Microwave ovens,   UHF TV,   FM radio,   AM
lamps   police radar,   cellular   VHF TV   radio
satellite stations   telephones

(a)

400 nm   500   600   700

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Problem: Calculate the wavelength, in meters, of radiation with a frequency of $1.18 \times 10^{14} \text{ s}^{-1}$.

What region of the electromagnetic spectrum is this?

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

$$\lambda \quad = \quad \frac{3.00 \times 10^8 \, \frac{m}{s}}{1.18 \times 10^{14} \, s^{-1}} \qquad = 2.54 \times 10^{-6} \text{ m} \qquad 1 \text{ nm} = 10^{-9} \text{ m}$$

$$= 2540 \text{ nm}$$

This is in the infrared region.

Particle-like Properties of Electromagnetic Radiation: The Planck Equation

Quantized Energy Levels

Pre-1900, classical physics assumed that atoms and molecules could *emit* (or *absorb*) **any arbitrary amount** of radiant energy – but this did **not** explain some experimental *observations* concerning radiation emission from some heated solids.

Planck in 1900 said that atoms and molecules could emit (or absorb) energy only in discrete quantities, like small packages or bundles.

Planck gave the name quantum to *the smallest **quantity** of energy that can be emitted (or absorbed) in the form of electromagnetic radiation.*

The energy *E* of a single quantum of energy is given by

$$\textbf{E} \quad = \quad \textbf{h}\nu \quad = \quad \frac{\textbf{hc}}{\lambda}$$

Planck's constant, $h = 6.626 \times 10^{-34}$ Js

According to quantum theory, energy is always emitted in integral multiples of $h\nu$; ($h\nu$, 2 $h\nu$, 3 $h\nu$ . . .), but never, for example, 1.67 $h\nu$ or 4.98 $h\nu$.

At the time Planck presented his theory, he could **not** explain **why** energies should be fixed or quantized in this manner.

Problem: Determine the energy emitted in the previous problem, of radiation with a frequency of 1.18×10^{14} s^{-1}.

$$E \quad = \quad h\nu \quad = \quad (6.626 \times 10^{-34} \text{ J·s}) (1.18 \times 10^{14} \text{ s}^{-1})$$
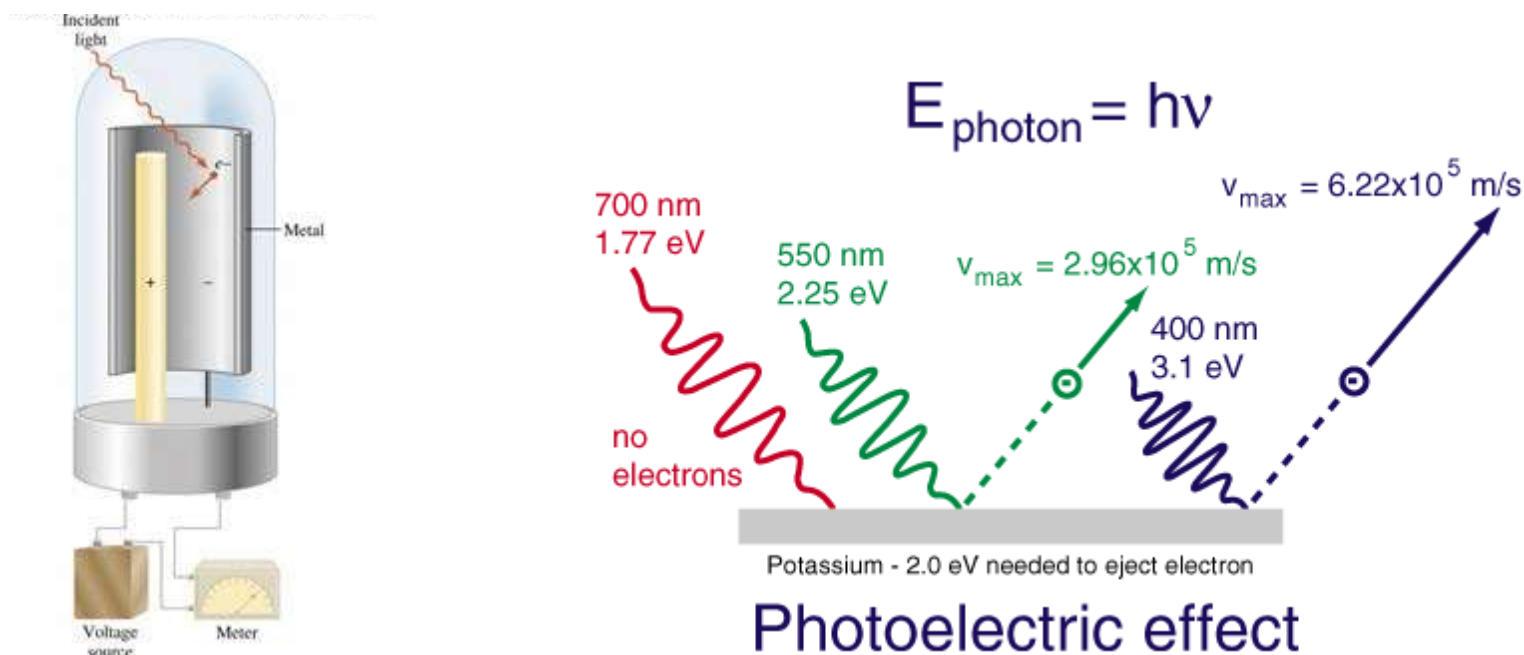
$$= \quad 7.82 \times 10^{-20} \text{ J}$$

Can also express energies in kJ·mol^{-1}

$$7.82 \times 10^{-20} \text{ J} \quad \times \quad \frac{6.022 \times 10^{23}}{\text{mol}} \quad \times \quad \frac{\text{kJ}}{1000 \text{ J}} \quad = 47.1 \ \frac{\text{kJ}}{\text{mol}}$$

Photoelectric effect

Five years after Planck's quantum theory, Einstein in 1905 described the photoelectric effect (or *photoemission*).

This is the production (or not) of electrons when *light* is *shone* onto a *material*. Electrons emitted in this manner can be called photoelectrons.

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

$v_{max} = 6.22 \times 10^5 \text{ m/s}$

700 nm
1.77 eV

550 nm
2.25 eV

$v_{max} = 2.96 \times 10^5 \text{ m/s}$

400 nm
3.1 eV

no
electrons

Potassium - 2.0 eV needed to eject electron

Photoelectric effect

According to *classical electromagnetic* (wave) theory, this effect can be attributed to the transfer of energy from the light to an electron. An alteration in either the intensity or wavelength of light would induce changes in the *rate* of *emission* of *electrons* from the metal. Furthermore, according to this theory, a sufficiently *dim* light would be expected to show a *time lag* between the *initial* shining of its light and the subsequent *emission* of an electron.

However, the experimental results did **not** correlate with either of the two predictions made by classical theory.

In reality, electrons are *only* dislodged by the impingement of photons that *reach* (or exceed) a *threshold frequency* (energy). Below that threshold, no electrons are emitted from the metal regardless of the light intensity or the length of time of exposure to the light.

To make sense of the experimental fact that light can eject electrons even if its *intensity* is *low*, Einstein proposed that a beam of light is **not** a wave propagating through space, but rather a *collection* of *discrete wave packets* (photons), each with energy hν. This shed light on Planck's previous discovery of the Planck relation ($E = h\nu$) linking energy (E) and frequency (ν) as arising from quantization of energy.

The (kinetic) energy of the *ejected* electron is equal to the energy in, minus however much energy it takes to get the *electron* away from the *material*.

$$KE = h\nu - \Phi$$ Where Φ is the work function of the metal (the *binding energy* of the electron that must be <u>overcome</u> in order to *liberate* the electron).

The main conclusion is that light travels in packets or as **particles** called photons, with energy hν.

But electromagnetic radiation (light) is a **wave**…

$\Rightarrow$ the wave-particle **duality** of light.

Bohr's model

The Rutherford–Bohr model or Bohr model, introduced by Niels Bohr in 1913, depicts the atom as a small, positively charged nucleus surrounded by electrons that travel in circular orbits around the nucleus—similar in structure to the solar system, but with attraction provided by *electrostatic* forces rather than gravity.

The electron (*fixed*) orbits can only have **certain** energy values (quantized).

$$E_n \;=\; (-R_H)\,\frac{1}{n^2} \qquad n = 1, 2, 3, 4,...$$

R_H is the Rydberg constant for Hydrogen $= 2.18 \times 10^{-18}$ J.

As written, the energy is zero when the electron is away from nucleus; and is more *negative* the *closer* the electron is to the *attractive* nucleus.

$$E_\infty \;=\; (-2.18 \times 10^{-18} \text{ J})\,\frac{1}{\infty^2} \;=\; 0$$

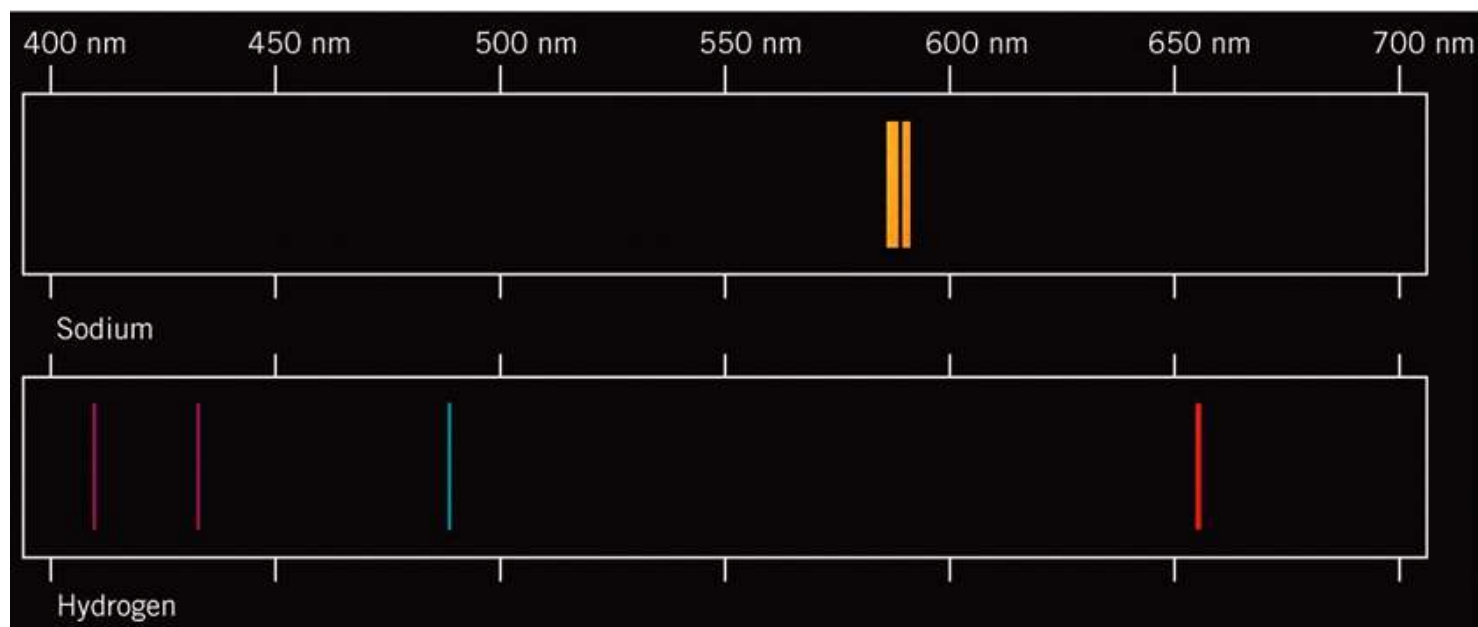$$\Delta E \;=\; E_f - E_i \quad = h\nu \;=\; R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$\text{So } \nu \;=\; \frac{\Delta E}{h} \qquad \text{and } \lambda = \frac{hc}{\Delta E}$$

Electronic Structure of an Atom

Atoms can absorb light.

More precisely, the electrons receive the energy and it boosts them
from a *lower* energy level to a *higher* energy level.
The lowest energy state is called the Ground State.

Any **higher** level is called an **Excited** state.

Excited states can emit light.

As the electron drops back to the *lower* energy level, there is an
emission of a photon.

excited state ———

+hν

ground state ———

——— excited state

−hν

——— ground state

Absorption of energy

Emission of light

$n = 4$ $n = 3$ $n = 2$ $n = 1$

$E = -b$
$E = -0.25b$
$E = -0.11b$
$E = -0.062b$

Some electromagnetic radiation sources generate **continuous** (*unbroken*) spectra, for example sunlight, incandescent light bulb, very hot metal rod, etc.
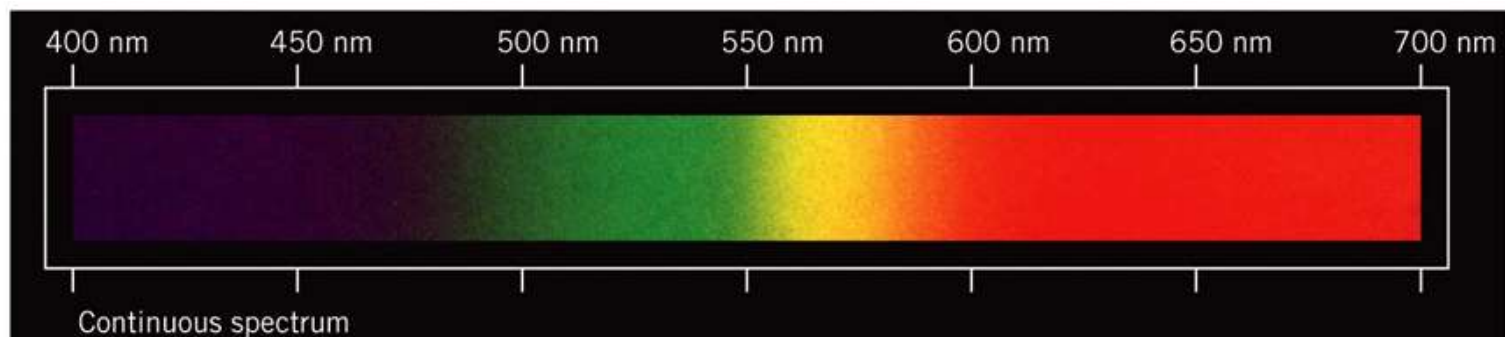
Whereas passing electricity through a (simple) gas under vacuum produces a **line** (*discontinuous*) spectrum, for example sodium vapor, or hydrogen gas.

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Problem: Calculate the wavelength of light emitted when an electron falls from the n = 3 to the n = 2 level in a hydrogen atom.

$$\Delta E \;=\; E_f - E_i \;\;=\; h\nu \;=\; R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

$$= \; (2.18 \times 10^{-18} \text{ J})\left(\frac{1}{3^2} - \frac{1}{2^2} \right)$$

$$= -3.03 \times 10^{-19} \text{ J} \qquad \text{meaning energy is emitted}$$

$$E = h\nu = \frac{hc}{\lambda} \qquad\qquad \text{so} \qquad \lambda = \frac{hc}{\Delta E} \;\; = \;\; \frac{(6.62 \times 10^{-34} \text{ J s})(3.00 \times 10^8 \frac{m}{s})}{3.03 \times 10^{-19} \text{ J}}$$

$$= \;\; 6.56 \times 10^{-7} \text{ m} \;\; = \;\; 656 \text{ nm (visible region, red)}$$

I am going to assume you know about PEDMAS (or BODMAS) orders of operations.

Electromagnetic Radiation and Atomic Spectra

Line spectra, also called atomic spectra are a series of discrete *lines* (or *wavelengths*) separated by blank areas.
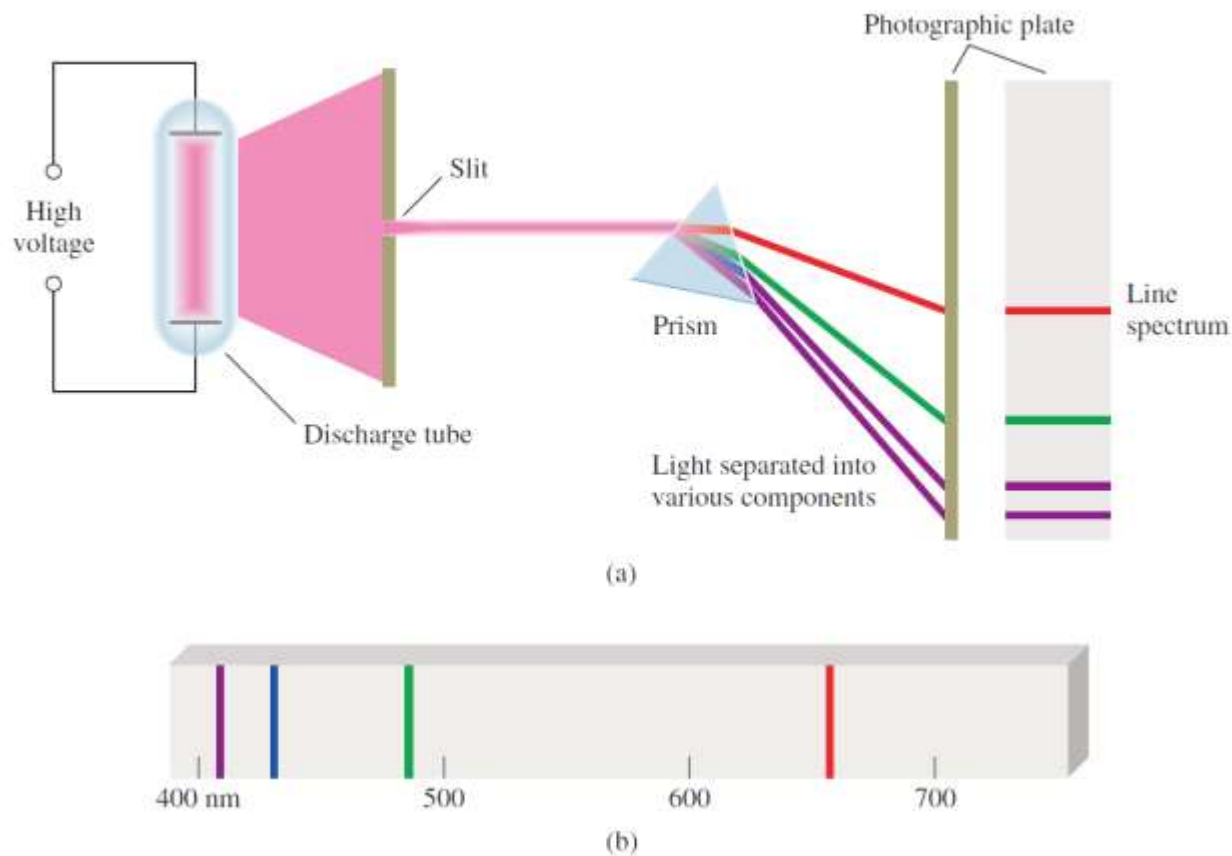
Line spectra are light emissions only at specific wavelengths.

Every element has a unique emission spectrum.

The experimental fact that there are only *certain* lines suggests quantization. Rydberg's equation explained these lines as transitions *from* one state/level/orbital *to* another.
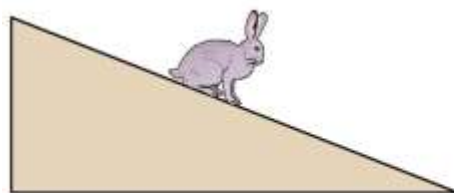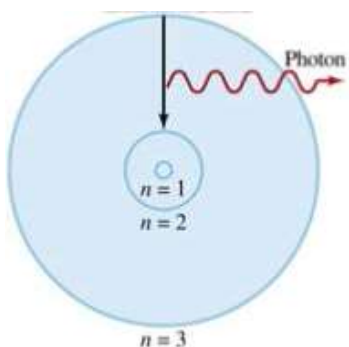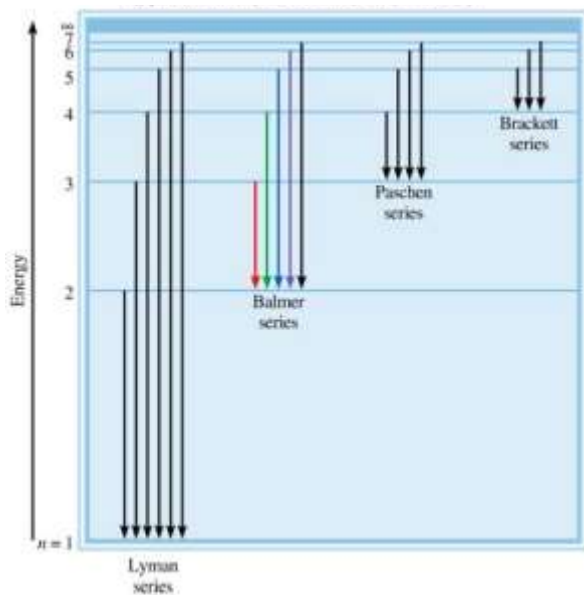

(a) Any potential energy allowed: energy values are *continuous*
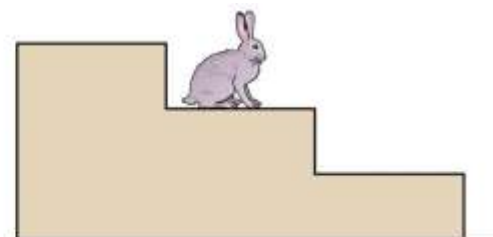
(b) Potential energy restricted: energy values are *discrete*

Emission lines of Hydrogen

Hydrogen emits several groups of lines (wavelengths).

This experiment suggests that the energy of (an atom's) electrons in orbitals can only take certain values (quantized).

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Wave-like Properties of Matter: the de Broglie Equation

The Wave Behavior of Matter

For the next 10 years scientists struggled with this (seemingly correct) idea that electrons seemed to be restricted to orbiting a nucleus at certain **fixed** distances.

In 1924, de Broglie suggested that if light (waves) can behave as a stream of particles, then perhaps particles can have wave-like properties.

The de Broglie's equation relates the mass and speed of the particle to its wavelength.

$$E = mc^2 \qquad E = h\nu = \frac{hc}{\lambda} \qquad \text{So} \quad mc^2 = \frac{hc}{\lambda}$$

$$(c = \lambda\nu)$$

$$\lambda = \frac{hc}{mc^2} = \frac{h}{mc}$$

The de Broglie wavelength of *something* with mass **m**, and velocity **v**:

notice this is v (velocity), not ν (frequency)

$$\lambda = \frac{h}{mv} \qquad \text{or} \qquad v = \frac{h}{m\lambda}$$

This is the (mathematical) **connection** between waves and particles.

(You get longer wavelengths for smaller masses, so this becomes increasingly important for smaller entities).

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He proposed that an electron bound to a nucleus can be described as a standing wave.

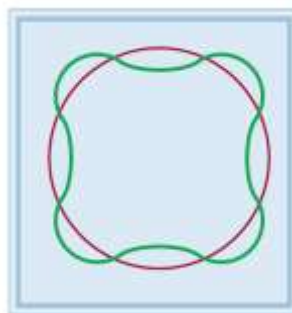For a standing wave (in a box), it must fit in the space exactly, which requires length $l = n\frac{\lambda}{2}$

where n is an integer.
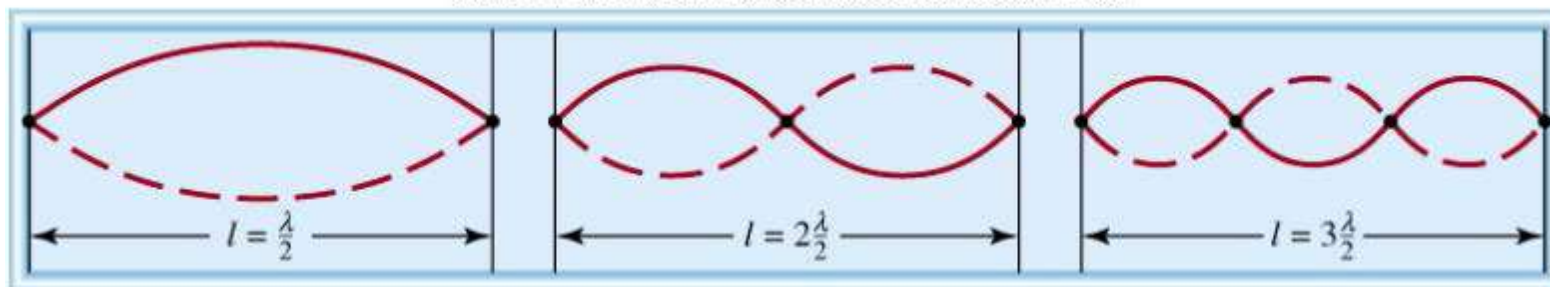
Electron orbits are circles, the circumference of an allowed orbit is $2\pi r$, then since the circumference of the orbit must be equal to an integral number of wavelengths:

$$2\pi r = n\lambda$$

Diffraction

Shortly after de Broglie introduced his equation, in 1937 Davisson and Germer in the United States, and Thomson in England demonstrated that electrons do indeed possess wave-like properties.

By directing a beam of electrons through a thin piece of gold foil, Thomson obtained a set of concentric rings on a screen, similar to the pattern observed when X- rays (which are *waves*) were used.

X-ray and electron diffraction patterns


(a)   (b)
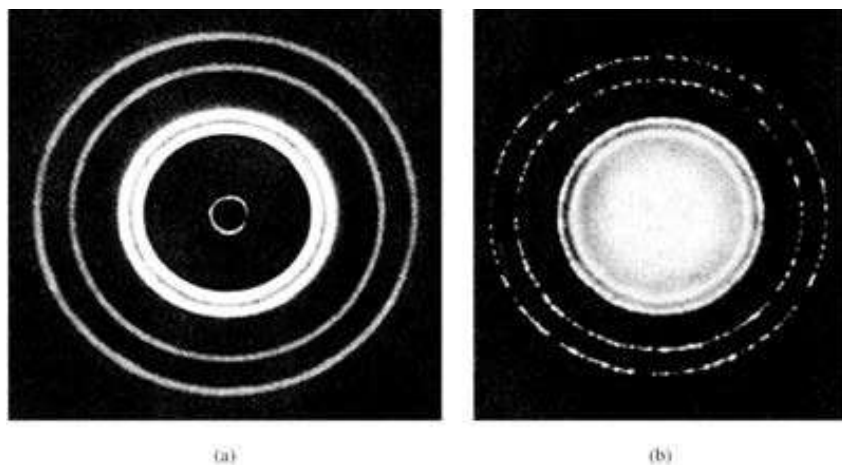
These **X-ray** and **electron** diffraction patterns from aluminum foil are similar since they both have **wave** properties.

One of the most important properties of waves is that they "interfere" with other waves…

Waves interfere with other waves.

Such as colored lights, or electrons in the double slit experiment.

Amplitude

Wave amplitudes add.

Wave amplitudes cancel to give zero amplitude.
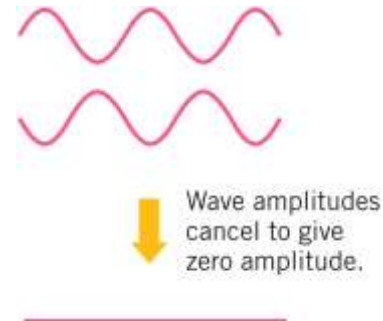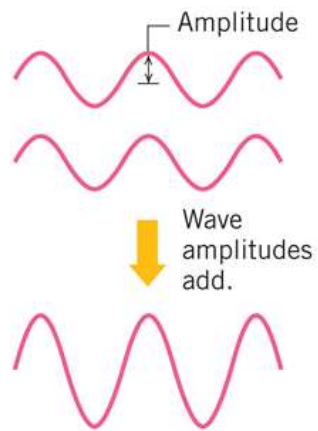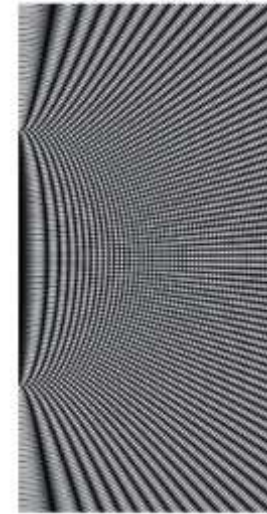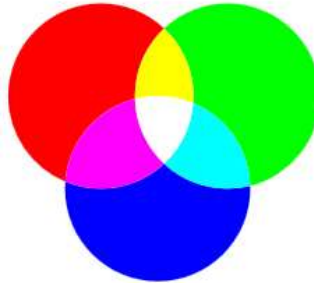
Waves can interfere *constructively* (in phase)…   …or *destructively* (out of phase).

Problem: What is the de Broglie wavelength of a 145 g baseball with a velocity of 90 mi/hr (40 m/s)?

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J s}}{(145 \text{ g}) (40\frac{m}{s})} \quad \text{x} \quad \frac{1000 \text{ g}}{1 \text{ kg}} \qquad \text{Note: } J = \frac{\text{kg m}^2}{s^2}$$

$$= 1.1 \times 10^{-34} \text{ m} \qquad \text{(undetectable size)}$$

Problem: What is the de Broglie wavelength of an electron (mass = 9.11×10^{-31} kg) traveling at 1/1000 of the speed of light (3.00×10^{8} m/s)?

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J s}}{(9.11 \times 10^{-31} \text{ kg}) (3.00 \times 10^{5}\frac{m}{s})}$$

$$= 2.42 \times 10^{-9} \text{ m} \quad \text{(Subatomic particles have measurable wavelengths)}$$

Quantum Mechanics and the Heisenberg Uncertainty Principle

Heisenberg

If you describe an electron as a wave, you run into some problems, such as how do you exactly define the position of the electron (*wave*).

In 1927, Heisenberg described the problem by stating it is inherently **impossible** to know *simultaneously* both the exact momentum (**mv**) of the electron and its exact location (**x**) in space.

$$\Delta x \, \Delta mv \; \geq \; \frac{h}{4\pi}$$

Where Δ means the "uncertainty" in measuring the location, or momentum.

So the *more precisely* you know the location, the *less precisely* you know the momentum, and vice versa.

Wave Functions and Quantum Numbers

Quantum Mechanics and Atomic Orbitals

In 1926, Schrödinger formulated an *equation* that describes the behavior and energies of submicroscopic particles in general, an equation analogous to Newton's laws of motion for macroscopic objects.

The Schrödinger equation incorporates both particle behavior, in terms of mass m, and wave behavior, in terms of a wave function ψ (psi), which depends on the *location* in space of the system (such as an *electron* in an *atom*).

The wave function itself has **no** direct physical meaning. However, the probability of finding the electron in a certain region in space is proportional to the square of the wave function, ψ^2.

The use of probability density and electron density – **likelihood** of finding an electron at that location, somewhat sidesteps the problems raised in the Heisenberg Uncertainty Principle.

Schrödinger's equation began a new era in physics and chemistry, quantum mechanics.

(Schrödinger's wave equation states when the Hamiltonian **operator**, **H**, acts on a certain wave function ψ, and the result is proportional to the same wave function ψ, then ψ is a *stationary state*, and the proportionality constant, **E**, is the energy of the state ψ :

$$\hat{H}\psi = E\psi \qquad \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Where **V** is a potential energy function).

Orbitals and Quantum Numbers

The complete solution to Schrodinger's equation for *the hydrogen atom* yields a set of wave equations and *corresponding* energies.

These wavefunctions are called orbitals.

An atomic orbital is a *mathematical function* that describes the *wave-like behavior* of an *electron* in an atom.

Quantum mechanics uses **three** quantum numbers **n**, *l*, and **m**$_l$, to describe an orbital.

1. Principal quantum number, n, can have *integer* values of 1, 2, 3 and so forth.

   As n *increases* the orbital becomes *larger* and *increases* in *energy*.

2. Azimuthal quantum number, *l*, can have values from (n–1) to 0, for each value of n.

   This quantum number gives the orbital its shape (the *angular momentum quantum number*).

Value of *l*	0	1	2	3	4	5
Letter used (*Name of Orbital*)	s	p	d	f	g	h

3. Magnetic quantum number, m$_l$ can have *integer* values between *l* and –*l*, including zero.

   This quantum number describes the *orientation* of the *orbital* in *space*.

The collection of orbitals with the *same value* of n is called an electron shell.

The set of orbitals with the *same* n **and** l values is called a subshell.

Each subshell is designated by a *number* (the value of n) and a *letter* (s, p, d, or f, corresponding to the value of l)

E.g.   2s subshell has   n = 2, $l = 0$

4f subshell has   n = 4, $l = 3$.

(Two) Restrictions on the possible values of the quantum numbers.

1.   The shell with the principal quantum number n will consist of exactly n subshells.

n = 1 has 1 subshell

n = 2 has 2 subshells

n = 3 has 3 subshells, etc.

2. Each subshell consists of a *specific* number of *orbitals*.

Each *orbital* corresponds to a different allowed value of m_l.

    For a given value of l there are $(2l + 1)$ allowed values for m_l, ranging from l to $-l$.

each s ($l = 0$) subshell consists of one orbital $2(0)+1 = 1$

each p ($l = 1$) subshell consists of three orbitals $2(1)+1 = 3$

each d ($l = 2$) subshell consists of five orbitals $2(2)+1 = 5$

In summary:

    n = principal quantum number; all orbitals with same n are in the same shell.

    l = secondary (azimuthal) quantum number; divides shells into subshells.

    m_l = magnetic quantum number; divides subshells into *individual* orbitals.

Orbitals are described by the three quantum numbers n, l and m_l.

Summary of Relationships among the Quantum Numbers n, ℓ, m_ℓ

Value of n	Value of ℓ	Value of m_ℓ	Subshell	Number of 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

l can have values from (n−1) to 0, for each value of n.

m_l can have *integer* values between l and –l, including zero.

The Shapes of Orbitals: Representations of Orbitals

**The s orbitals** (one per n)

• spherically symmetrical.

• probability function approaches zero as the distance from the nucleus *increases*.
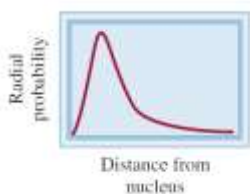
• 2s orbital has a node (region where the probability, ψ^2, goes to *zero*).

• 3s orbital has two nodes.

• As **n** *increases*, the electron is more likely to be *farther* from the nucleus.
The *size* of the orbital increases as n increases.


Relative sizes of the s orbitals:
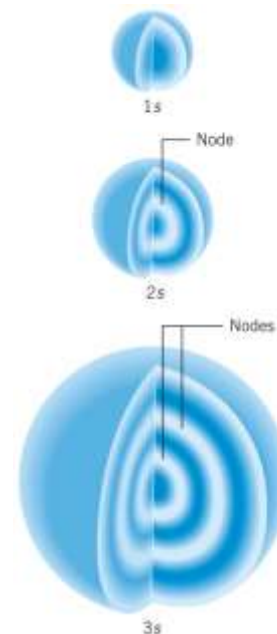
We *designate* a *boundary* of *probability* for the electron, and make that the shape of the orbital (e.g. 90% *chance* of the electron being found inside).
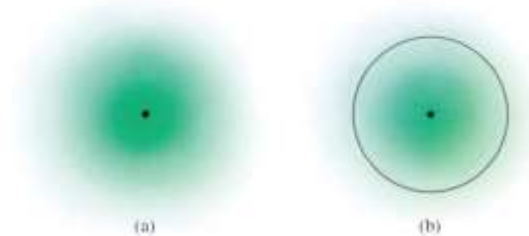
The p orbitals (3 per n)

    • **not** spherically symmetrical

    • all p orbitals have nodes at the *nucleus*

    • on either side of the node there are lobes

    • n = 2 has three p orbitals; all the same *size*, but one *oriented* along each axis: p_x, p_y, p_z.

    • p orbitals *increase* in size as **n** *increases*.
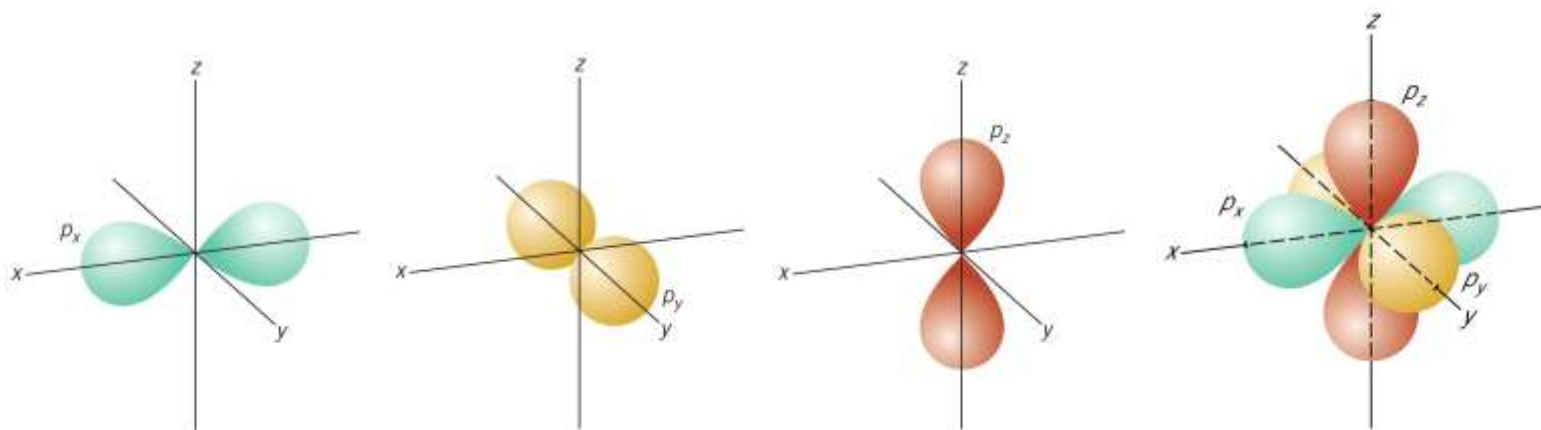
3 individual p orbitals   superimposed

The d orbitals (5 per n)

- four of the d ($l = 2$) orbitals have "*four-leaf clover*" shapes.

- they lie primarily in a plane: d_{xy}, d_{xz}, d_{yz}, with lobes between axes, whereas the $d_{x^2 - y^2}$ lies in the x-y plane along the axes.

- the d_{z^2} orbital has two lobes along the z axis and a "*doughnut*" in the xy plane. It has the same energy as the other four d orbitals.
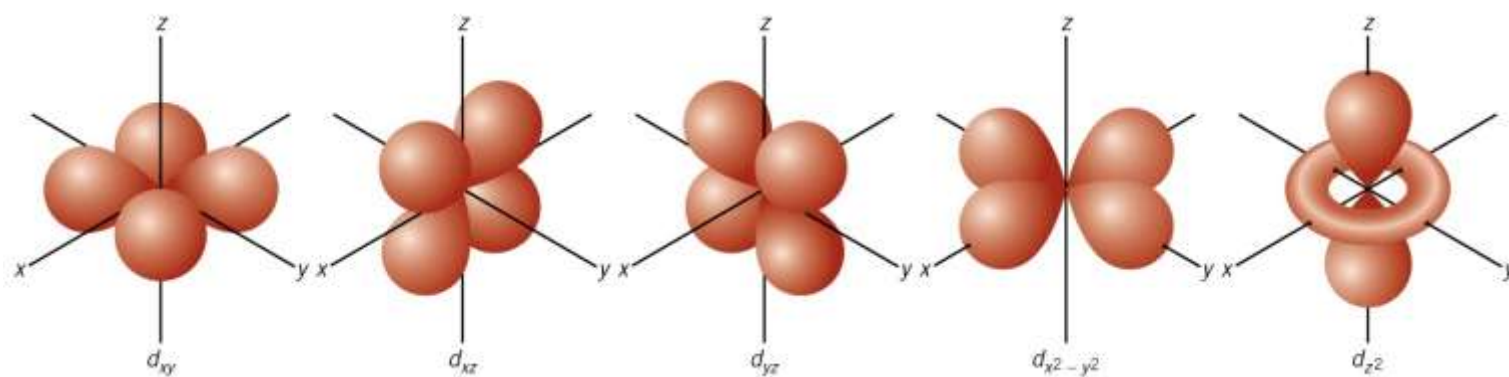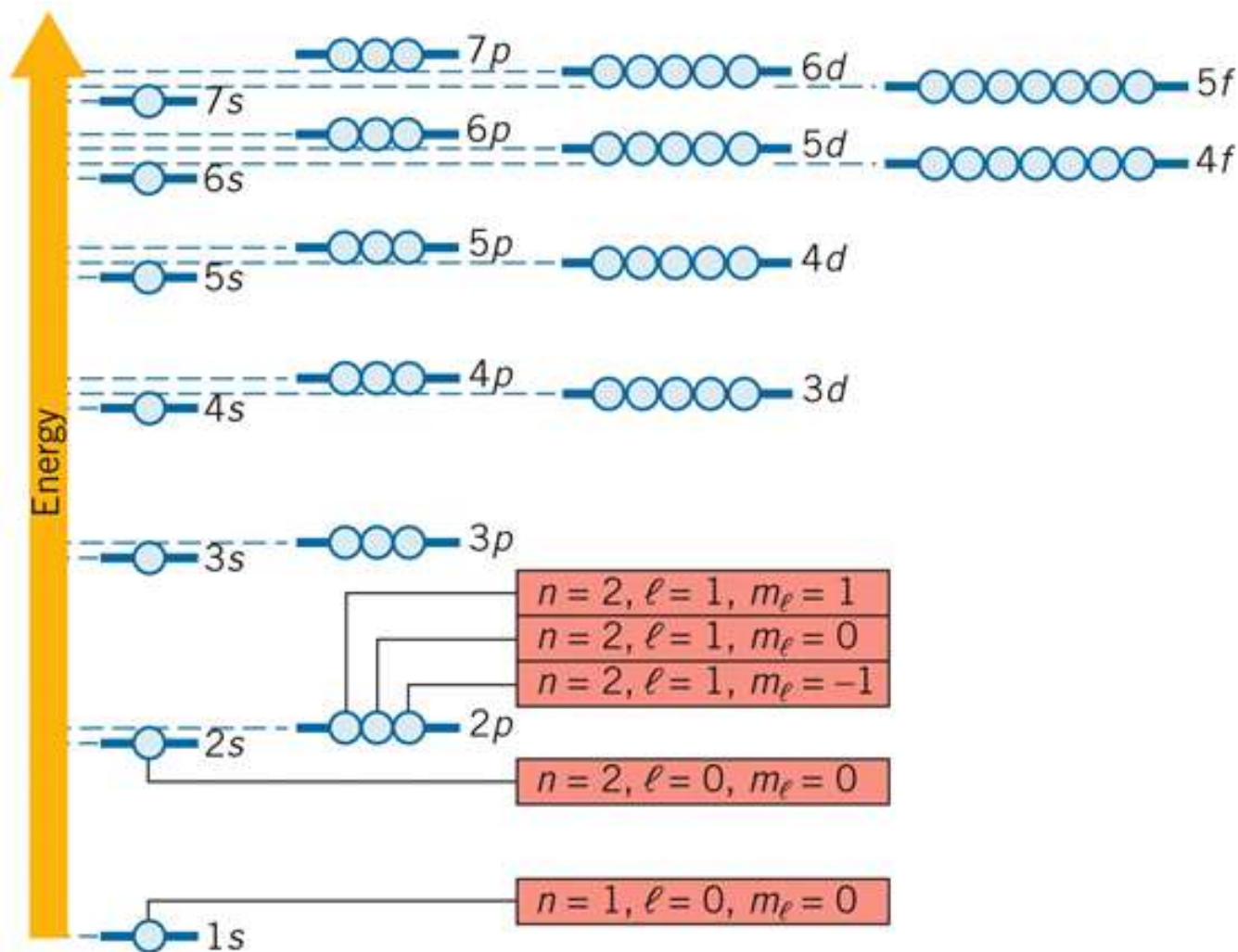

5 individual p orbitals

The f orbitals (7 per n)

The f orbitals ($l = 3$) are even more complicated than the d orbitals.

$5z^3 - 3zr^2$ $5xz^2 - xr^2$ $zx^2 - zy^2$ xyz

$y^3 - 3yx^2$ $5yz^2 - yr^2$ $x^3 - 3xy^2$
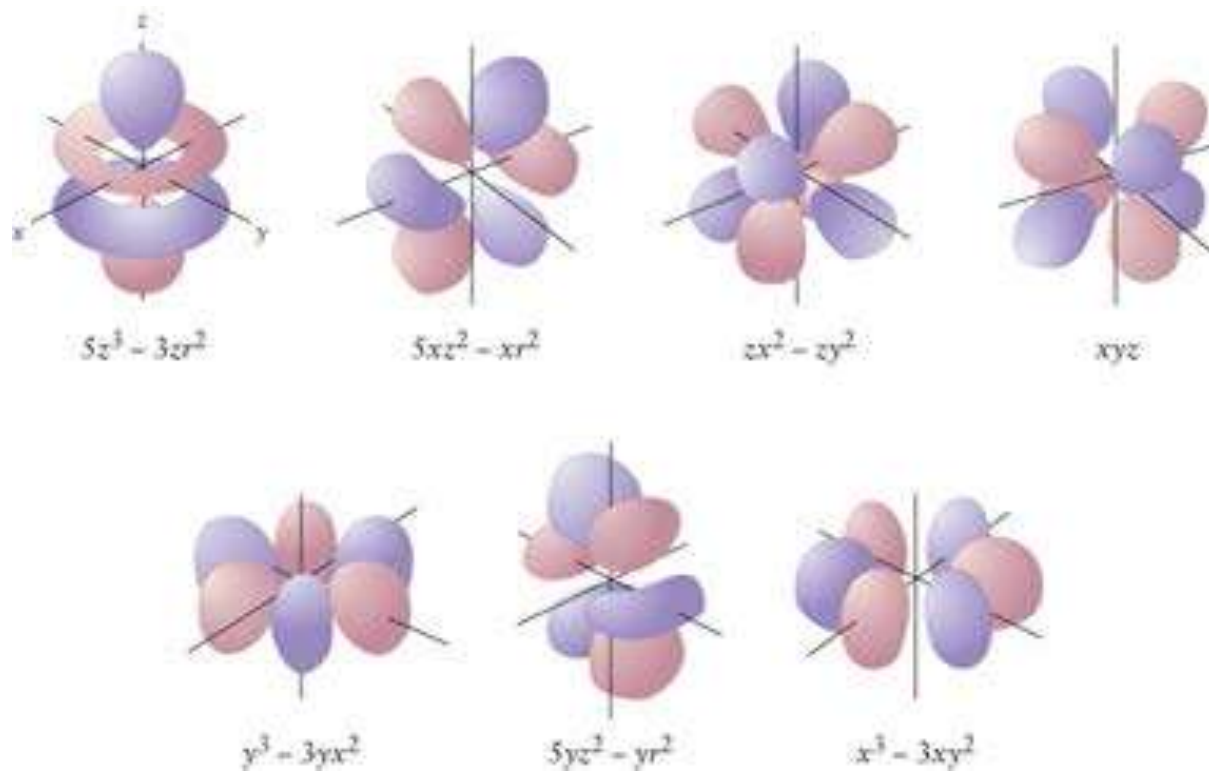
Relative Energies of Orbitals of (*Multielectron*) Atoms

Electron Spin and the Pauli Exclusion Principle

Electron Spin Quantum Number

How do electrons *populate* the available orbitals?

A new (4th) quantum number called the Electron Spin Quantum Number, $\mathbf{m_s}$, is introduced.

It has two possible values: $+\frac{1}{2}$ and $-\frac{1}{2}$ (often referred to as spin *up* and spin *down*)

The Pauli Exclusion Principle states that **no** two electrons (in the *same* atom) can have the same set of four quantum numbers (n, l, m_l, and m_s).

An orbital can hold a *maximum* of **two** electrons, and they must have *opposite* spins.

Diamagnetism and Paramagnetism

When two electrons in the same orbital have different spins we say they are spin paired = diamagnetic

- Sample not attracted to magnetic field (slight repulsion)

- Magnetic effects tend to cancel each other

When two electrons in are different orbitals with the same spin they can be spin unpaired = paramagnetic

- Sample attracted to a magnetic field

- *More* unpaired electrons lead to a *stronger* attraction to a magnet
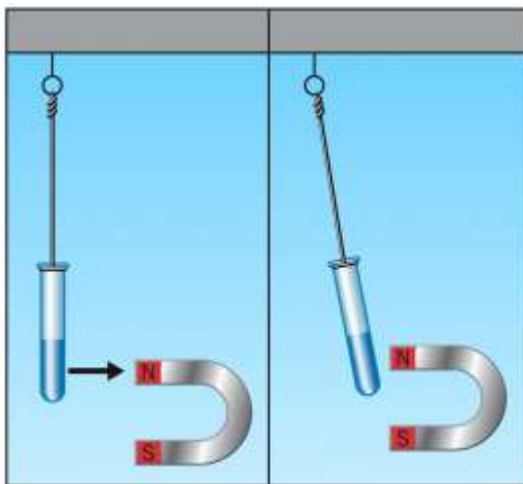
We can measure the extent of the attraction, which provides information about the number of unpaired spins.

**Orbital Energy Levels in Many-Electron Atoms**

In *many-electron* atoms, the energy levels differ.

E.g. the 2s subshell is lower in energy than the 2p subshell.

Any electron density between the nucleus and the electron of interest will *reduce* the nuclear charge acting on that electron.

The *net positive charge* attracting the electron is called the effective nuclear charge, $\mathbf{Z_{eff}}$.

$$\mathbf{Z_{eff} = Z - S}$$
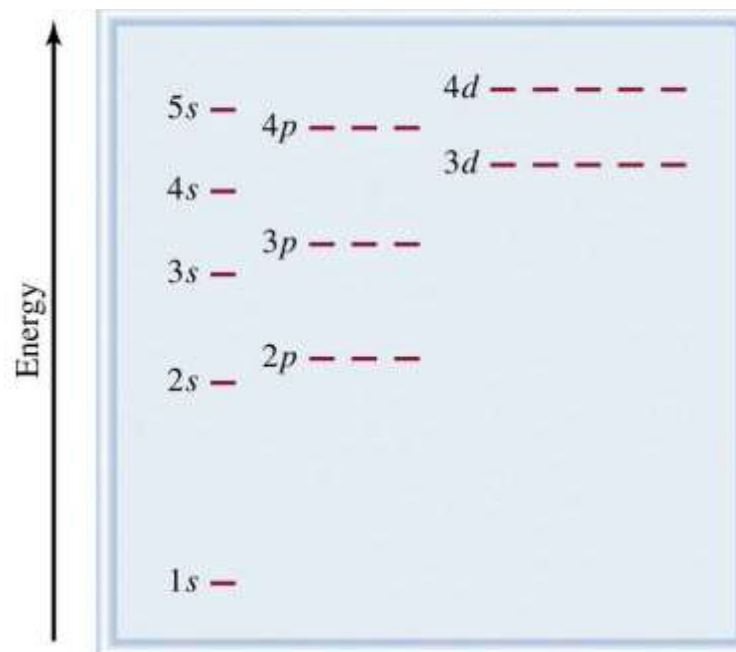
Where $\mathbf{Z}$ = number of protons in nucleus; $\mathbf{S}$ = the average number of electrons between the nucleus and the electron in question.

The energy of the orbital (*electron*) depends on the Effective Nuclear Charge and Shielding.

Lithium

2– core

3+

If an electron were here it would feel a net charge of about 1+.
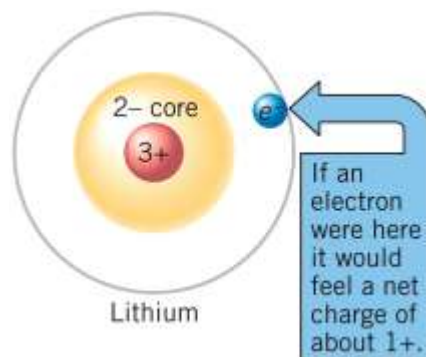
This figure shows the *radial probability* of different orbitals, even though the 2s is on average further from the nucleus than the 2p, notice the region close to the nucleus for the 2s.

The electron density *closer to the nucleus* is greater for the 2s than the 2p.

The 2s experiences *less* shielding by the 1s than the 2p does – so if 1s has electrons then 2s is lower in energy than 2p.

"penetrating power" $s > p > d > f$

1s

2p

2s

Radial probability

Distance from nucleus
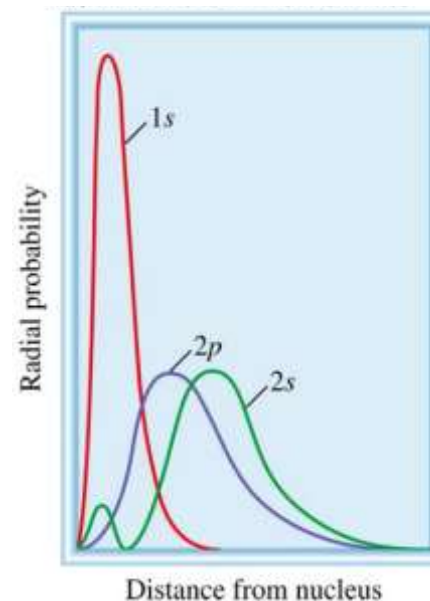
Energies of Orbitals

In a many-electron atom, for a given value of n, Z_{eff} decreases with increasing value of l.

In a many-electron atom, for a given value of n,   the energy of an orbital increases with increasing value of l.

$$s < p < d$$

Orbitals of a subshell have the same energy.

Orbitals with the *same energy* are said to be degenerate.

Electron Configurations of Multielectron Atoms

The way in which the electrons are distributed among the various orbitals of an atom is called its electron configuration.

The aufbau principle (1920) says we add electrons *one at a time*, to the *lowest* available orbital, until we have added the correct number of electrons.

Orbital diagram: each orbital is represented by a box (or circle) and each electron is represented by a half arrow (or arrow).

Nitrogen $1s^2 \, 2s^2 \, 2p^3$

Li

1s   2s

Li

$1s^2$ $2s^1$

1s   2s   2p
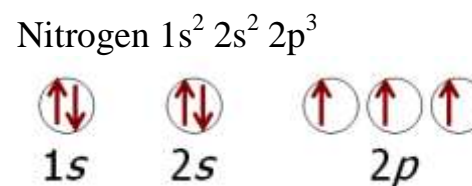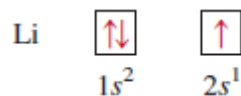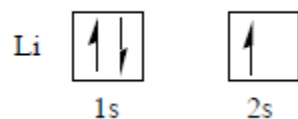
Electrons having *opposite* spins are paired, when they are in the same orbital.

The most stable, or ground state, electron configuration of an atom is that in which the electrons are in the lowest possible energy states. (Higher energy arrangements are called excited states).

Hund's rule: (1927) for degenerate orbitals, the *lowest* energy is attained when the number of *electrons* with the **same** *spin* is maximized.

Orbitals of a subshell will fill with electrons of the **same** spin first, *then*, with electrons of **opposite** spin.

Electron Configuration of the First 10 Elements

H   ↑
    $1s^1$

He ↑↓
    $1s^2$

Li ↑↓ ↑
    $1s^2$ $2s^1$

Be ↑↓ ↑↓
    $1s^2$ $2s^2$

B   ↑↓ ↑↓ ↑ □ □
    $1s^2$ $2s^2$ $2p^1$

C   ↑↓ ↑↓ ↑ ↑ □
    $1s^2$ $2s^2$ $2p^2$

N   ↑↓ ↑↓ ↑ ↑ ↑
    $1s^2$ $2s^2$ $2p^3$

O   ↑↓ ↑↓ ↑↓ ↑ ↑
    $1s^2$ $2s^2$ $2p^4$

F   ↑↓ ↑↓ ↑↓ ↑↓ ↑
    $1s^2$ $2s^2$ $2p^5$

Ne ↑↓ ↑↓ ↑↓ ↑↓ ↑↓
    $1s^2$ $2s^2$ $2p^6$
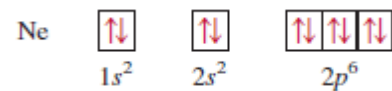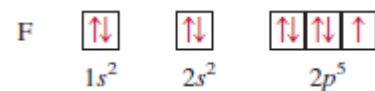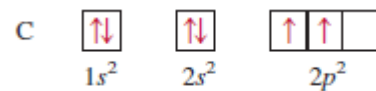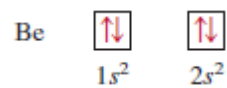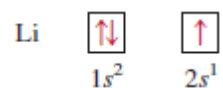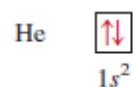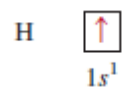
The filling of the 2p subshell is complete at **neon**, which has a *stable configuration* with *eight* electrons (an octet) in the outermost shell.

Sodium has a single electron beyond the stable configuration of neon. We abbreviate the electron configuration of sodium as follows:

$$Na \quad = \quad [Ne]\ 3s^1$$

which is the same as $\qquad 1s^2\ 2s^2 2p^6\ 3s^1$

Since $[Ne] = \qquad 1s^2\ 2s^2 2p^6$

Similarly $\quad Li = [He]\ 2s^1$

Electrons in *subshells* not occupied in the nearest noble-gas element of *lower* atomic number are referred to as outer-shell electrons, or valence electrons.

The electrons in the *inner shells* are the core electrons.

All of the above applies for Periods (rows) 1, 2 and 3; for Period 4 and beyond it gets a little more involved…

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$Ar = 1s^2 \; 2s^2 2p^6 \; 3s^2 3p^6$

So is K $\qquad 1s^2 \; 2s^2 2p^6 \; 3s^2 3p^6 3d^1$

Or $\qquad\qquad 1s^2 \; 2s^2 2p^6 \; 3s^2 3p^6 \; 4s^1$? $\qquad\qquad$ ☑
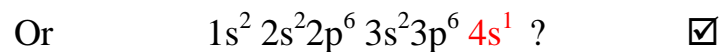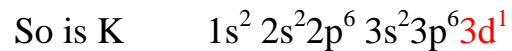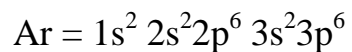
K has properties similar to **Na**. This suggests that the electron is in an s orbital.

This means that the 4s orbital is lower in energy than the 3d (*see earlier diagrams #30 and #33*).
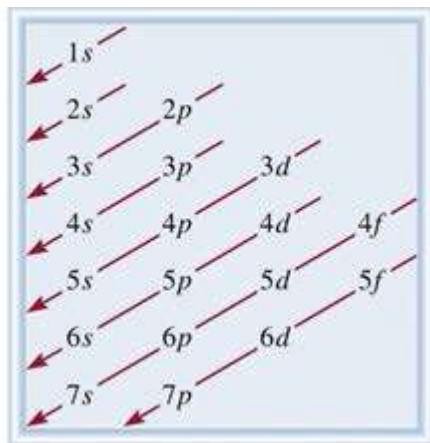
This is the *order* in which the atomic subshells are filled.

Start with the 1s orbital and move downward following the red arrow.

So 1s, 2s, 2p, 3s, 3p, 4s, 3d, ...

Electron Configurations and the Periodic Table

The periodic table is also a *guide* to the order in which orbitals are filled.

1s			1s
2s			2p
3s			3p
4s	3d		4p
5s	4d		5p
6s	5d		6p
7s	6d		7p

4f
5f

The classification of groups of elements in the periodic table according to the type of subshell being filled with electrons.

Notice these periodic occurrences:

All of Gp 1A are $\mathbf{ns^1}$ All of 3A are $\mathbf{ns^2\ np^1}$ All of 7A are $\mathbf{ns^2\ np^5}$

1A																	8A
	2A											3A	4A	5A	6A	7A	
		3B	4B	5B	6B	7B	8B		1B	2B							

E.g. $_{17}Cl = [Ne]\ 3s^2 3p^5$

$_{83}Bi = [Xe]\ 6s^2\ 4f^{14}\ 5d^{10}\ 6p^3$ $Xe = 54$

Outer electron Configuration for all the elements

1 / 1A																	18 / 8A
1 H $1s^1$	2 / 2A											13 / 3A	14 / 4A	15 / 5A	16 / 6A	17 / 7A	2 He $1s^2$
3 Li $2s^1$	4 Be $2s^2$											5 B $2s^22p^1$	6 C $2s^22p^2$	7 N $2s^22p^3$	8 O $2s^22p^4$	9 F $2s^22p^5$	10 Ne $2s^22p^6$
11 Na $3s^1$	12 Mg $3s^2$	3 / 3B	4 / 4B	5 / 5B	6 / 6B	7 / 7B	8	9 / 8B	10	11 / 1B	12 / 2B	13 Al $3s^23p^1$	14 Si $3s^23p^2$	15 P $3s^23p^3$	16 S $3s^23p^4$	17 Cl $3s^23p^5$	18 Ar $3s^23p^6$
19 K $4s^1$	20 Ca $4s^2$	21 Sc $4s^23d^1$	22 Ti $4s^23d^2$	23 V $4s^23d^3$	24 Cr $4s^13d^5$	25 Mn $4s^23d^5$	26 Fe $4s^23d^6$	27 Co $4s^23d^7$	28 Ni $4s^23d^8$	29 Cu $4s^13d^{10}$	30 Zn $4s^23d^{10}$	31 Ga $4s^24p^1$	32 Ge $4s^24p^2$	33 As $4s^24p^3$	34 Se $4s^24p^4$	35 Br $4s^24p^5$	36 Kr $4s^24p^6$
37 Rb $5s^1$	38 Sr $5s^2$	39 Y $5s^24d^1$	40 Zr $5s^24d^2$	41 Nb $5s^14d^4$	42 Mo $5s^14d^5$	43 Tc $5s^24d^5$	44 Ru $5s^14d^7$	45 Rh $5s^14d^8$	46 Pd $4d^{10}$	47 Ag $5s^14d^{10}$	48 Cd $5s^24d^{10}$	49 In $5s^25p^1$	50 Sn $5s^25p^2$	51 Sb $5s^25p^3$	52 Te $5s^25p^4$	53 I $5s^25p^5$	54 Xe $5s^25p^6$
55 Cs $6s^1$	56 Ba $6s^2$	57 La $6s^25d^1$	72 Hf $6s^25d^2$	73 Ta $6s^25d^3$	74 W $6s^25d^4$	75 Re $6s^25d^5$	76 Os $6s^25d^6$	77 Ir $6s^25d^7$	78 Pt $6s^15d^9$	79 Au $6s^15d^{10}$	80 Hg $6s^25d^{10}$	81 Tl $6s^26p^1$	82 Pb $6s^26p^2$	83 Bi $6s^26p^3$	84 Po $6s^26p^4$	85 At $6s^26p^5$	86 Rn $6s^26p^6$
87 Fr $7s^1$	88 Ra $7s^2$	89 Ac $7s^26d^1$	104 Rf $7s^26d^2$	105 Db $7s^26d^3$	106 Sg $7s^26d^4$	107 Bh $7s^26d^5$	108 Hs $7s^26d^6$	109 Mt $7s^26d^7$	110 Ds $7s^26d^8$	111 Rg $7s^26d^9$	112 $7s^26d^{10}$	113 $7s^27p^1$	114 $7s^27p^2$	115 $7s^27p^3$	116 $7s^27p^4$	(117)	118 $7s^27p^6$

58 Ce $6s^24f^15d^1$	59 Pr $6s^24f^3$	60 Nd $6s^24f^4$	61 Pm $6s^24f^5$	62 Sm $6s^24f^6$	63 Eu $6s^24f^7$	64 Gd $6s^24f^75d^1$	65 Tb $6s^24f^9$	66 Dy $6s^24f^{10}$	67 Ho $6s^24f^{11}$	68 Er $6s^24f^{12}$	69 Tm $6s^24f^{13}$	70 Yb $6s^24f^{14}$	71 Lu $6s^24f^{14}5d^1$
90 Th $7s^26d^2$	91 Pa $7s^25f^26d^1$	92 U $7s^25f^36d^1$	93 Np $7s^25f^46d^1$	94 Pu $7s^25f^6$	95 Am $7s^25f^7$	96 Cm $7s^25f^76d^1$	97 Bk $7s^25f^9$	98 Cf $7s^25f^{10}$	99 Es $7s^25f^{11}$	100 Fm $7s^25f^{12}$	101 Md $7s^25f^{13}$	102 No $7s^25f^{14}$	103 Lr $7s^25f^{14}6d^1$

Some Anomalous Electron Configurations

These rules apply *almost* all of the time, but you should be aware of some *exceptions*.

E.g.   **Cr** should be   [Ar] $4s^2\,3d^4$ but actually is   [Ar] $4s^1\,3d^5$

[Ar]   ↑   ↑ ↑ ↑ ↑ ↑

$4s^1$ $3d^5$

Also, **Cu** should be   [Ar] $4s^2\,3d^9$ but is actually   [Ar] $4s^1\,3d^{10}$

[Ar]   ↑   ↑↓ ↑↓ ↑↓ ↑↓ ↑↓

$4s^1$ $3d^{10}$

The difference arises since there is an *enhanced stability* associated with half or fully filled subshells.

A similar effect is observed for Silver and Gold.