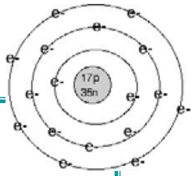
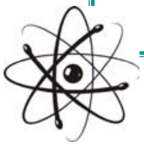
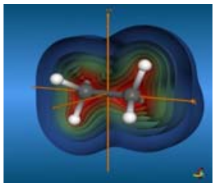
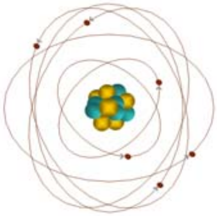


Chapter 6

Quantum Theory and the Electronic Structure of Atoms







Preview

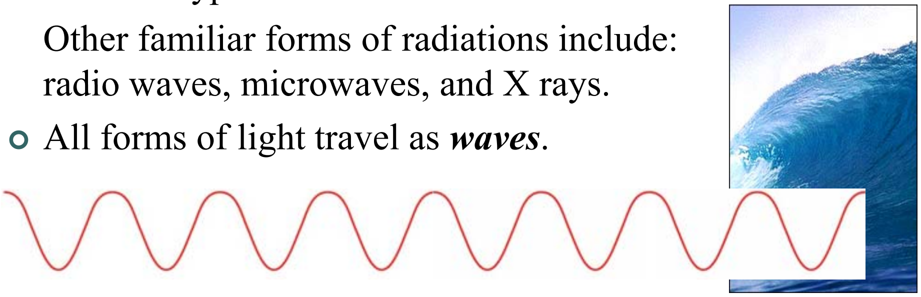
- Nature of light and electromagnetic radiation.
- Quantum theory.
- Atomic spectrum for hydrogen atom.
- The Bohr model.
- Quantum numbers.
- Shapes and energies of atomic orbitals.
- Electron configuration and periodic table.

Chapter 6 Section 1

The Nature of Light

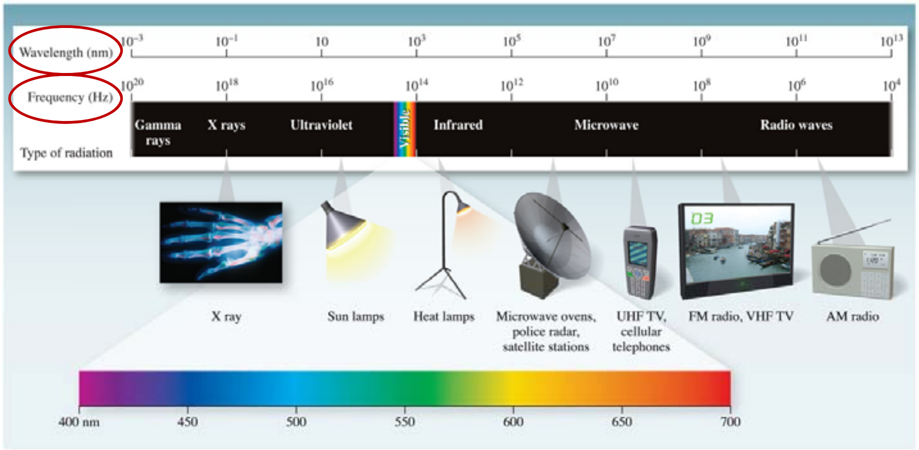
- Visible light (red, yellow, blue, etc.) is a small part of the electromagnetic spectrum.
- ***Electromagnetic spectrum*** includes many different types of radiation.

  Other familiar forms of radiations include: radio waves, microwaves, and X rays.
- All forms of light travel as ***waves***.



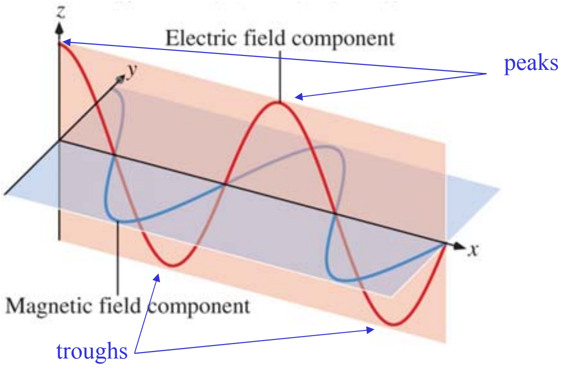
Chapter 6 Section 1

Electromagnetic Spectrum



Properties of Waves

- Energy travels in space in the form of electromagnetic (EM) radiations, which have ***electric*** component and ***magnetic*** component.



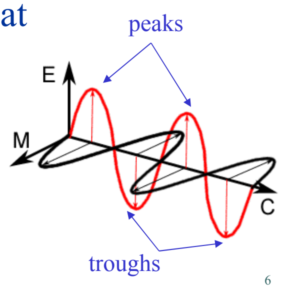
Properties of Waves

- Waves are characterized by their:
  - **Wavelength (λ)**

    Distance between two consecutive peaks or troughs in a wave.
  - **Frequency (ν)**

    Number of waves per second that pass a given point.
  - **Amplitude (A)**

    The vertical distance from the midline to the top of the peak or the bottom of the trough.



Chapter 6 Section 1

Properties of Waves

- All types of EM radiations travel at speed of light (***c***).
- ***λ*** and ***v*** are inversely related.

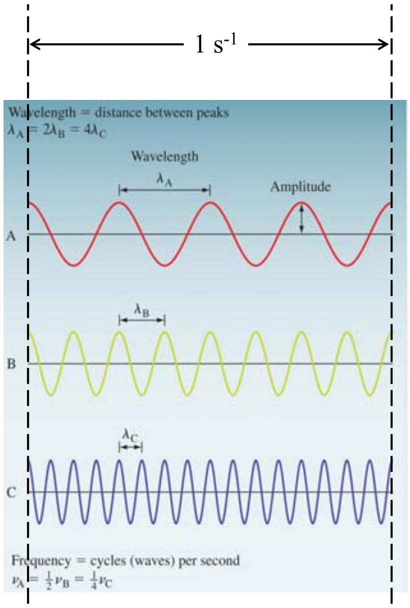
λ α $1/v$ => $\lambda = c\,(1/v)$

$\boxed{c = \lambda\, v}$

$c = 2.9979 \times 10^8$ m/s

⇨ λ is given in a unit length (m).

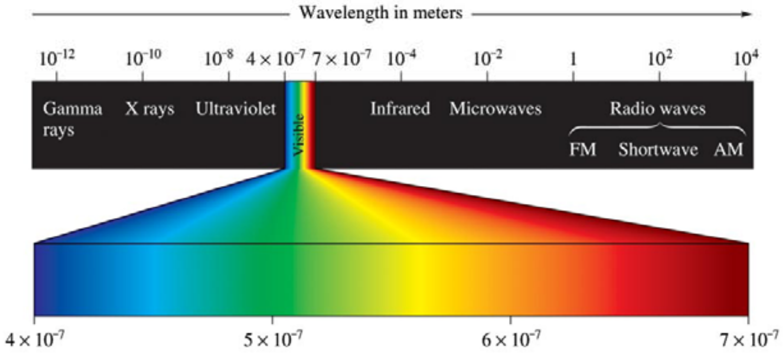
⇨ v is cycles per 1 second (s^{-1}), or *Hertz*.



Dr. A. Al-Saadi

Chapter 7 Section 1

Classification of Electromagnetic Radiation



Higher frequencies ←

Shorter wavelengths

Higher Energy

Lower frequencies →

Longer wavelengths

Lower Energy

Dr. A. Al-Saadi

Frequency of a Visible Light

Strontium salt $Sr(NO_3)_2$ is what gives the red brilliant color in the firework

- The emitted light is of about 650 nm wavelength. Calculate the frequency.

Wavelength

$c = \lambda \nu$ ← Frequency

Speed of light

$\nu = c/\lambda$

$c = 2.9979\times10^{8}$ m/s

$\lambda = 6.50$ nm $= 6.50\times10^{-9}$ m

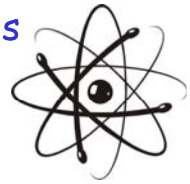
$\nu = (2.9979\times10^{8}$ m/s$) / (6.50\times10^{-9}$ m$)$

$= 4.61\times10^{14}$ s^{-1}(or Hz)

Quantum Theory

The beginning of the 20th century, physicists found that **classical physics** was **not** successful to explain the properties of matter at the subatomic level. Many experiments supported this argument.

- Blackbody radiation "Planck".
- The photoelectric effect "Einstein".
- Spectrum of the hydrogen atom "Bohr".



Chapter 6 Section 2

Energy of Blackbody Radiation

- ***Blackbody*** emits EM radiation over a wide range of wavelengths.
- Attempts to understand the energy of blackbody radiations based on ***classical physics*** were not successful. Classical physics assumed that radiant energy is *continuous*. *Look for "ultraviolet catastrophe"*
- *Thinking outside the box.*
- In 1900, Max Plank proposed that the radiant energy could only be emitted or absorbed in discrete quantities, each of which is called ***quantum***.

Chapter 6 Section 2

Planck: Energy is Quantized

- It was the birth of ***modern "or quantum" physics***.
  - **Planck:** the energy of a single quantum of energy is:

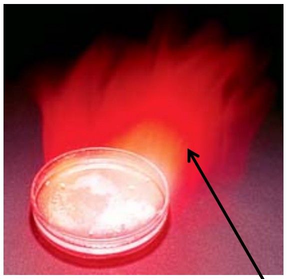
$$\boxed{E = h\nu}$$

- E : energy of a single quantum in joules (J)
- h : Planck's constant = 6.626×10^{-34} J·s
- ν : Frequency in s^{-1}

- Planck proposed that absorptions or emissions of energy take place in only *whole-number multiples* of quantities "quanta", each of which has the size of $h\nu$.

Chapter 6 Section 2

Energy of a Visible Light



$\nu = 4.61\times10^{14}$ Hz

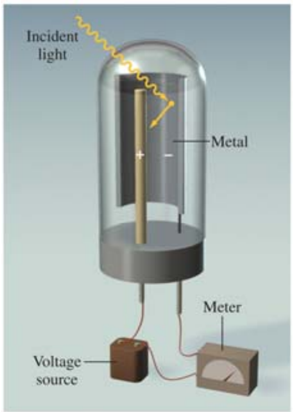
$$E = h\nu$$
$$= 6.626 \times 10^{-34}\ \text{J.s} \times 4.61\times10^{14}\ \text{s}^{-1}$$
$$= 3.05\times 10^{-19}\ \text{J}$$

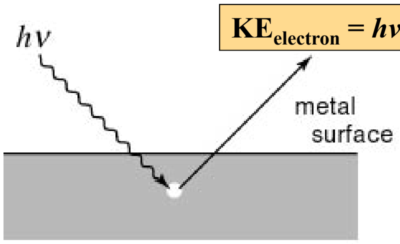
A sample of $Sr(NO_3)_2$ emitting light at 650 nm can lose energy only in increments of 3.05×10^{-19} J (the size of the energy packet).

Chapter 6 Section 2

The Photoelectric Effect

- When a light beam strikes a metal surface. What will happen??

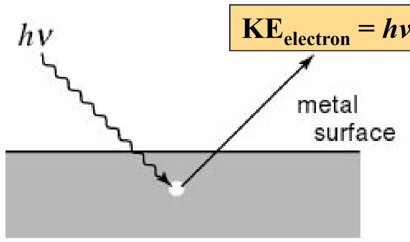




$$\mathbf{KE}_{\text{electron}} = h\nu - \underbrace{h\nu_0}_{W\ \text{“Work function”}} = \tfrac{1}{2} mv^2$$

Electrons are ejected from the surface of the metal exposed to the light beam of at least a certain minimum frequency, called the ***threshold frequency*** **(ν_0)**.

The Photoelectric Effect



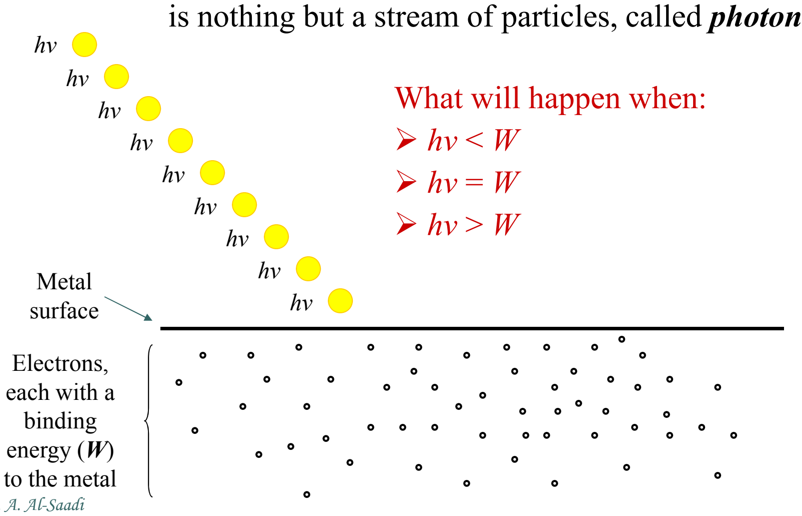
$$\mathrm{KE}_{\mathrm{electron}} = h\nu - \underbrace{h\nu_0}_{W} = \tfrac{1}{2}\, mv^2$$

“Work function”

- It was observed that:
  - The ***number of electrons*** ejected was proportional to the ***intensity*** of the incident light, not to its frequency.
  - The ***energy of the electrons*** ejected was proportional to the ***frequency*** of the incident light, not to its intensity.

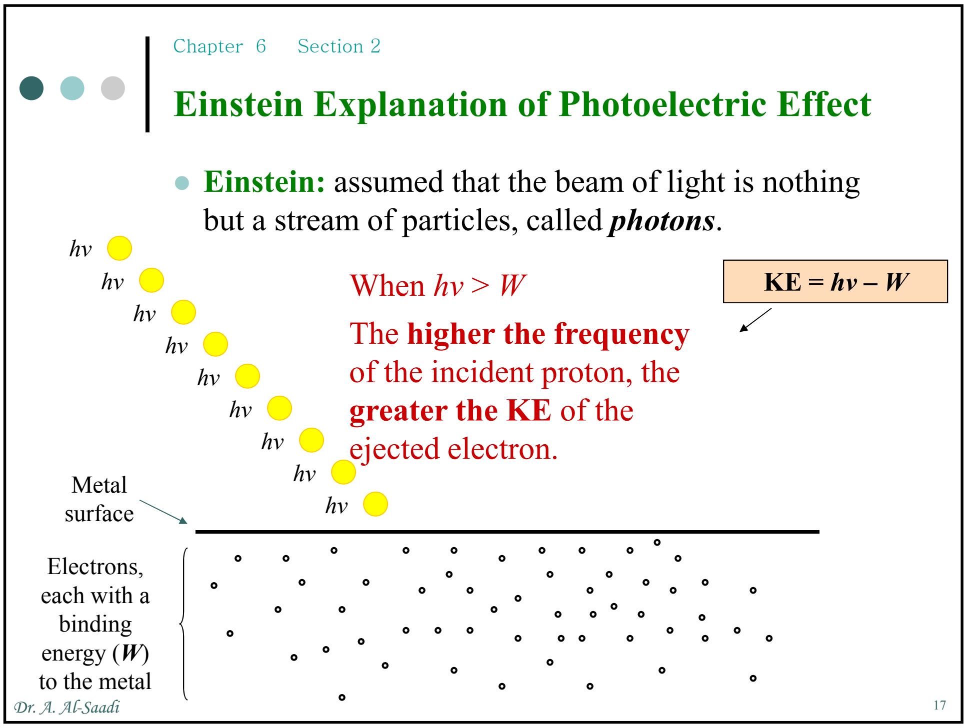
Einstein Explanation of Photoelectric Effect

- **Einstein:** In 1905, he assumed that the beam of light is nothing but a stream of particles, called ***photons***.



What will happen when:

- $h\nu < W$
- $h\nu = W$
- $h\nu > W$



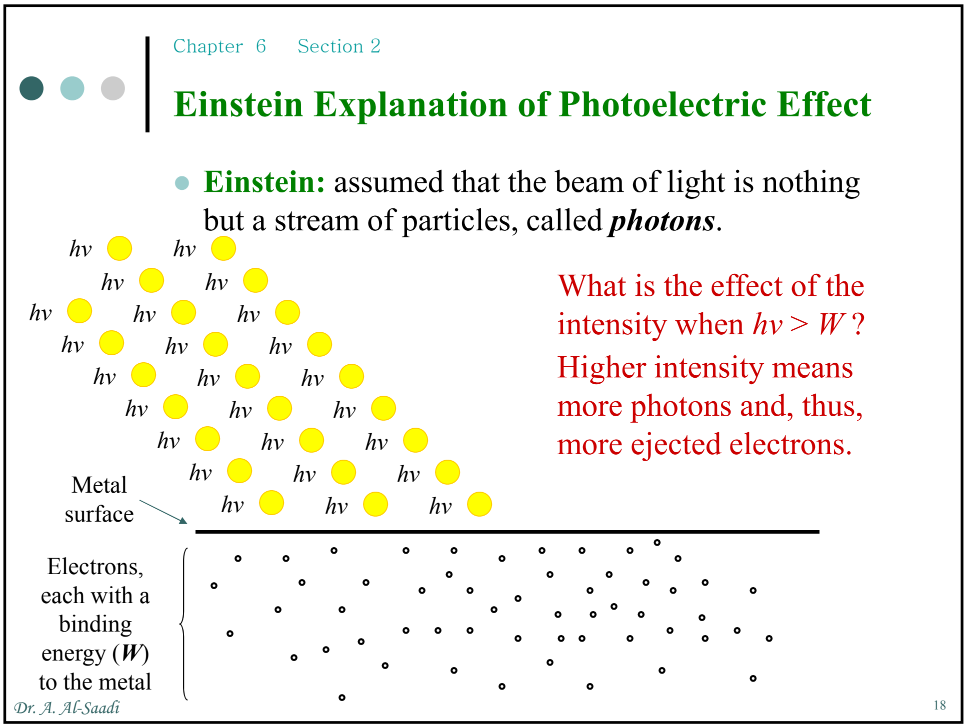
Einstein Explanation of Photoelectric Effect

- **Einstein:** assumed that the beam of light is nothing but a stream of particles, called ***photons***.

When $hv > W$

The **higher the frequency** of the incident proton, the **greater the KE** of the ejected electron.

KE = $hv - W$



Einstein Explanation of Photoelectric Effect

- **Einstein:** assumed that the beam of light is nothing but a stream of particles, called ***photons***.

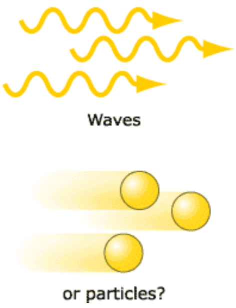
What is the effect of the intensity when $hv > W$?

Higher intensity means more photons and, thus, more ejected electrons.

Chapter 6 Section 2

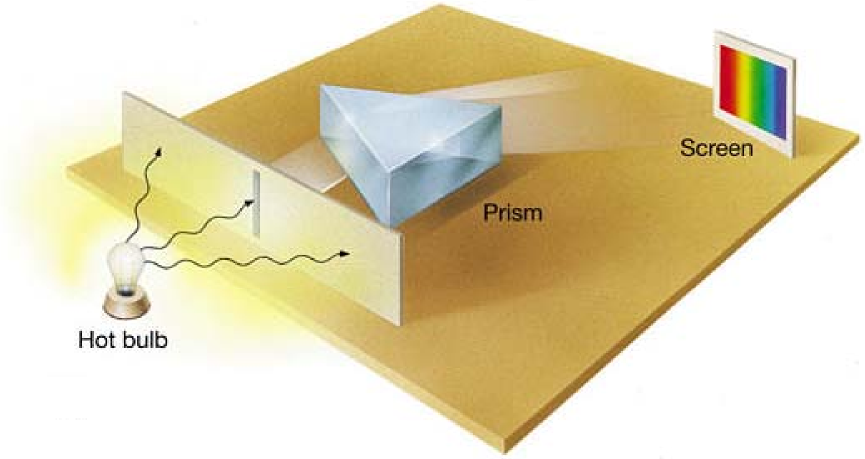
Dual Nature of Light

- Dilemma caused by this theory - is light a wave or particle?
- Conclusion: Light must have particle characteristics as well as wave characteristics
- Energy is quantized. It occurs only in discreet units (quanta) called ***photons***.
- EM radiation represents dual nature of light (wave and matter).



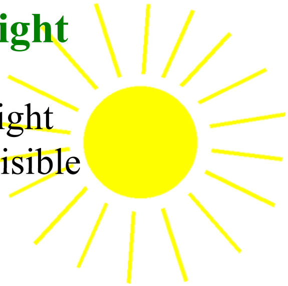
Chapter 6 Section 3

Continuous Spectrum of Light

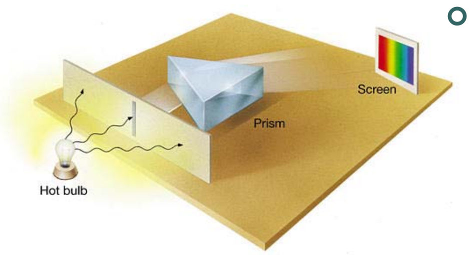


Chapter 6 Section 3

Continuous Spectrum of Light



- The ***continuous spectrum*** of white light shows the components of light “all visible wavelengths” as continuous colors.
- Continuous spectra are also know as ***emission spectra***.



- Can you think of other sources of emission spectra?
  - Kitchen stove.
  - Tungsten lamp.
  - Glowing a piece of iron.

Chapter 6 Section 3

Atomic Line Spectra

- Unlike sunlight, emission spectra of atoms give just few lines rather than giving all colors!

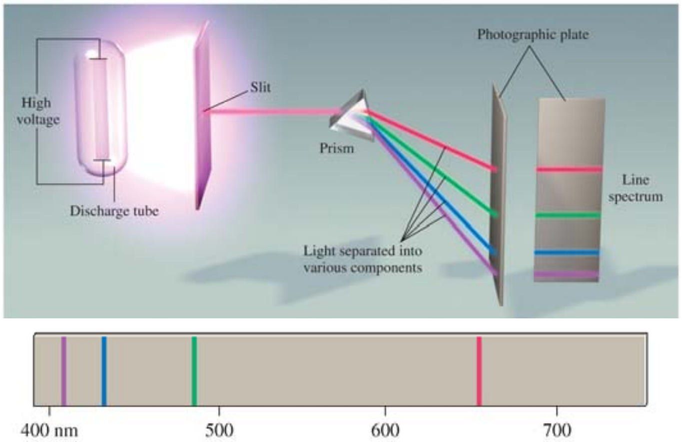
  These are called ***line spectra***.

  In other words, only *few wavelengths* are there.

- $$H_2(g) + \text{Energy} \longrightarrow H(g) + H(g)$$

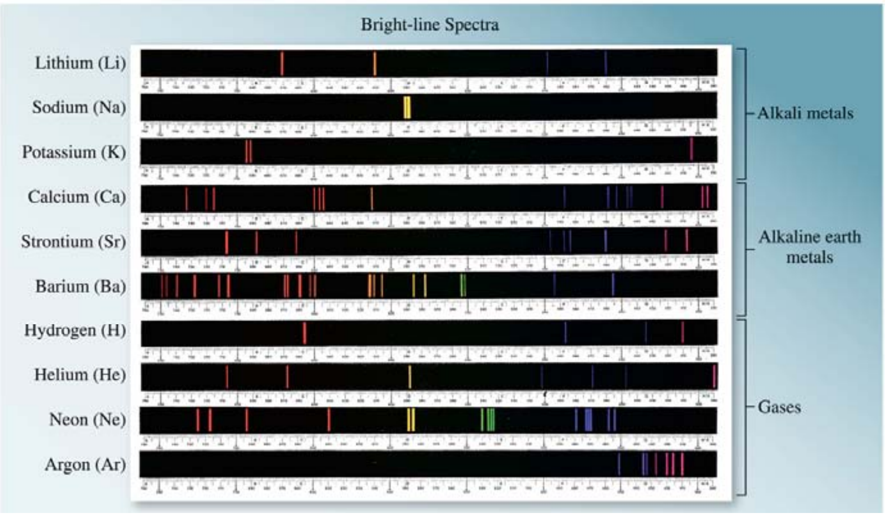
  H atoms are *excited* (having excessive energy). Then, this energy is released by emitting light of various wavelengths, known as “line spectrum” or “emission spectrum” of hydrogen.

The Atomic Spectrum of Hydrogen



The origin of the line spectra was a mystery until the revolution of the quantum theory.

Not only the H Atom Has a Line Spectrum!

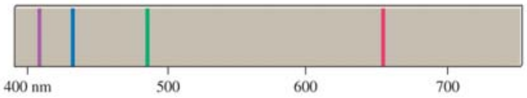


Rydberg Equation

- Balmer (initially) and Rydberg (later) developed the equation to calculate the wavelengths of **all spectral lines** in hydrogen.

$$\frac{1}{\lambda} = R_{\infty}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

- Rydberg constant (R_{∞}) = 1.097373×10^{7}m^{-1}.
- n_1 and n_2 are positive integers where $n_2 > n_1$.
- λ is wavelength in meter.



- The line spectrum of hydrogen has lines in the visible region and in the other regions.

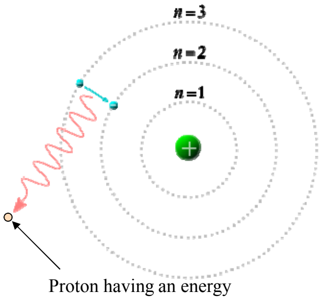
The Line Spectrum of Hydrogen

- **View of Classical Physics.**
  - For an electron rotating with a high speed around a nucleus *the centrifugal force* is just balanced by the *attraction force* to the nucleus.
  - A charged particle under acceleration should radiate energy *continuously*. Thus the electron inside the atom would quickly spiral towards the nucleus by radiating out energy in form of EM radiation and eventually collides nucleus.
  - This is not true!

The Line Spectrum of Hydrogen

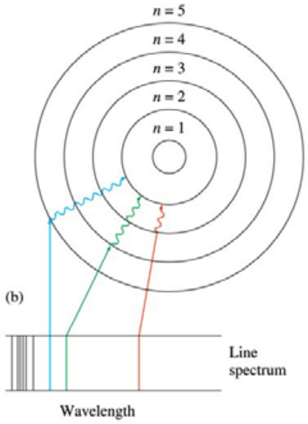
- **Niels Bohr.**
  - In 1913, Bohr postulated that the electron in the hydrogen model moves around the nucleus only in ***certain allowed circular paths*** or ***orbits***.
  - He assumed the electron radiates energy only at ***discrete quantities*** equivalent to the energy differences between these circular orbits.
  - The energies of the electron in the hydrogen atom is ***quantized***.

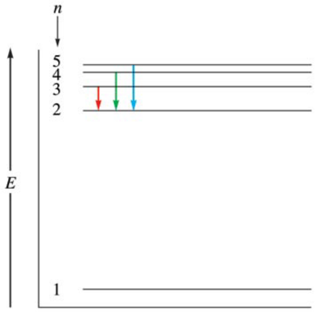
Bohr Model



Proton having an energy of E_3-E_2= hv

The Bohr Model





- Bohr was able to calculate the hydrogen atom energy levels obtained from the experiment.

$$E = -2.18\times10^{-18}\,\text{J}\left(\frac{Z^2}{n^2}\right)$$

- Each spectral line corresponds to a specific transition .

Chapter 6 Section 3

The Bohr Model

$$E = -2.18 \times 10^{-18}\,\mathrm{J}\left(\frac{Z^2}{n^2}\right)$$

E is the energy associated with the electron present at level n.

n is an integer indicating the level (orbit) number.

Z is the nuclear charge ($Z = 1$ for hydrogen atom).

- The negative sign means that the energy of the electron attracted to the nucleus is less than it would be if the electron had no interaction with nucleus ($n = \infty$).

  For $n = \infty$, $E = 0$

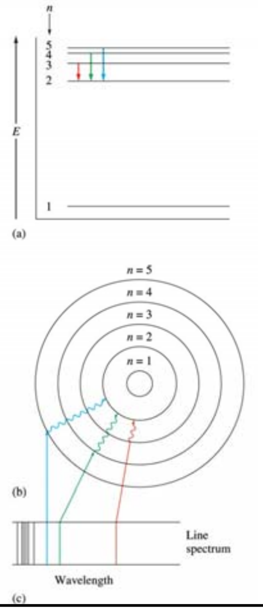
Chapter 6 Section 3

The Bohr Model

$$E = -2.18 \times 10^{-18}\,\mathrm{J}\left(\frac{Z^2}{n^2}\right)$$

- As the electron gets closer to the nucleus, E_n becomes larger in absolute value but also more negative.
- ***Ground state***: the lowest energy state of an atom.

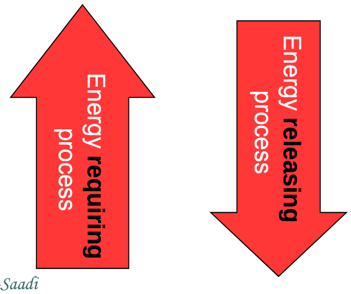
  Excited state: each energy state in which $n > 1$.
- An electron moving from the ground state to a higher exited states ***requires*** or ***absorbs*** energy; an electron falling from a higher to a lower state ***releases*** or ***emits*** energy.



Chapter 6 Section 3

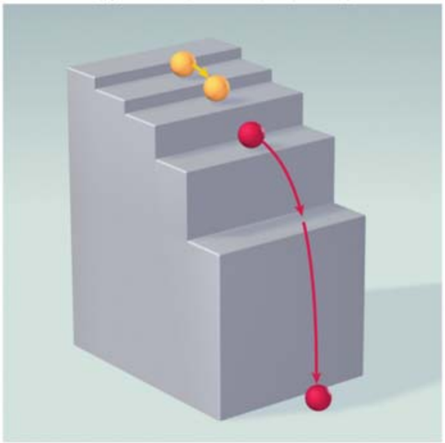
The Bohr Model

- The electron transition within quantized energy levels is similar to the movement of a tennis ball up or down a set of stairs.



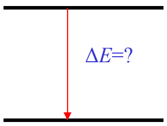
Energy **requiring** process

Energy **releasing** process



Chapter 6 Section 3

Application of Bohr Model



For $n = 6$: $$E_6 = -2.18\times10^{-18}\,\text{J}\left(\frac{(1)^2}{(6)^2}\right) = -6.050\times10^{-20}\,\text{J}$$

For $n = 1$: $$E_1 = -2.18\times10^{-18}\,\text{J}\left(\frac{(1)^2}{(1)^2}\right) = -2.178\times10^{-18}\,\text{J}$$

ΔE = energy of final state – energy of initial state

$= E_1 - E_6 = -\,2.117\times10^{-18}$ J

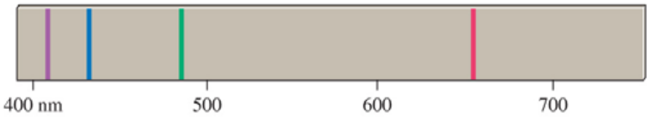
What is λ for the emitted photon (light)? $$\Delta E = \frac{hc}{\lambda}$$

Application of Bohr Model

- For an electron moving from one level (n_{initial}) to another level (n_{final}) in hydrogen atom:

$$\Delta E = h\nu = -2.18\times10^{-18}\,\text{J}\left(\frac{1}{n_{\text{final}}^2}-\frac{1}{n_{\text{initial}}^2}\right)$$

- **Bohr model is only applicable to the hydrogen atom.**



Application of Bohr Model

- Calculate the energy required to remove the electron from a hydrogen atom in its ground state.

$$\Delta E = -2.18\times10^{-18}\,\text{J}\left(\frac{1}{n_{\text{final}}^2}-\frac{1}{n_{\text{initial}}^2}\right)$$

Chapter 6 Section 3

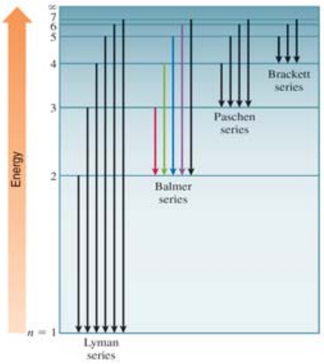
Emission Series in the Hydrogen Spectrum

TABLE 6.1 Emission Series in the Hydrogen Spectrum

Series	n_f	n_i	Spectrum Region
Lyman	1	2, 3, 4, . . .	Ultraviolet
Balmer	2	3, 4, 5, . . .	Visible and ultraviolet
Paschen	3	4, 5, 6, . . .	Infrared
Brackett	4	5, 6, 7, . . .	Infrared

- The hydrogen emission spectrum involves many electronic transitions with a wide range of wavelengths.

  The only visible ones are those of Balmer series.



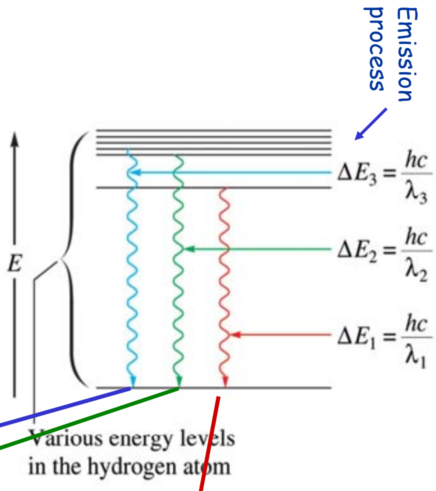
Chapter 6 Section 3

Balmer Series

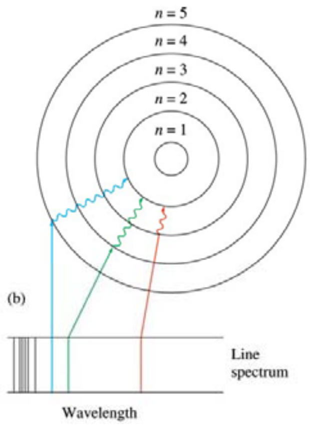
- The only visible lines in the hydrogen emission spectrum are those associated to Balmer series.

- Plank's equation:

  $\Delta E = hv = hc/\lambda$



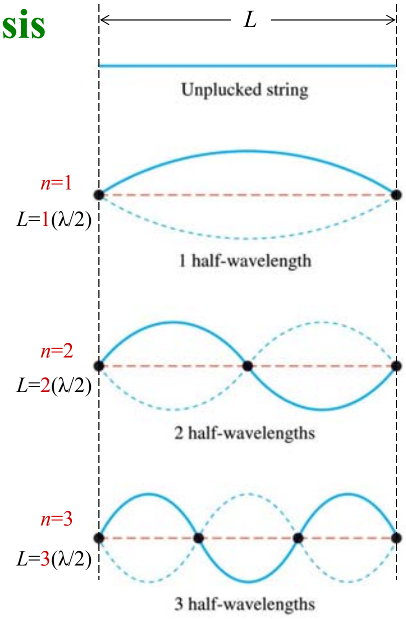
Wave Properties of Matter



- Bohr as well as physicists of his time could not explain why electrons were restricted to fixed distances around the nucleus
- In 1924, Louis de Broglie mentioned that if energy (light) can behave as a particle (photon), then why not to say that particles (electrons) could exhibit wave properties!

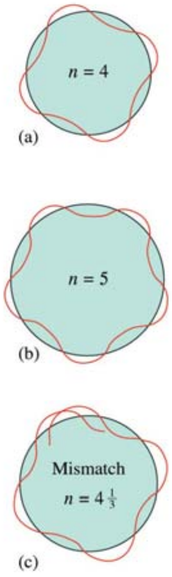
De Broglie Hypothesis

- De Broglie proposed that the electron bound to the nucleus behaves similar to a ***standing wave*** or a ***stationary wave***.
- There are some points called ***nodes*** (where the wave exhibits no motion at all, or the amplitude $A = 0$.)
- The length (L) of the string must be equal to a whole number (n) times one-half of the wavelength ($\lambda/2$).



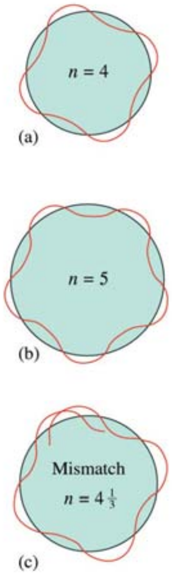
De Broglie Hypothesis

- Hydrogen electron in its path, or orbit, can be visualized as a *standing wave*.
- Only certain circular paths, such as (a) and (b), have circumferences into which a whole number of wavelength of standing electron waves will *fit constructively*.
- All other paths, such as (c), would build *destructively*, and the amplitudes of such paths quickly reduce to zero.
- This is in consistence with the fact that electron energies are *quantized*.



De Broglie Hypothesis

- De Broglie concluded that the energy of the electron in a hydrogen atom, if it behaves like a standing wave, must be ***quantized***.
- Waves can behave like particles and particles can exhibit wavelike properties.



Chapter 6 Section 4

De Broglie Equation

For a particle with velocity u:

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

(from Einstein equation)

Solving for λ:

$$\boxed{\lambda = \frac{h}{mu}}$$

- λ: de Broglie wavelength (m)
- m: mass (kg)
- u: velocity (m/s)

of a moving particle.

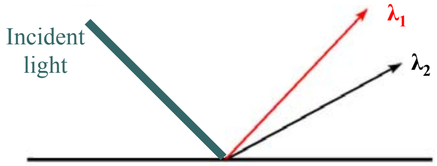
- Sample Problem

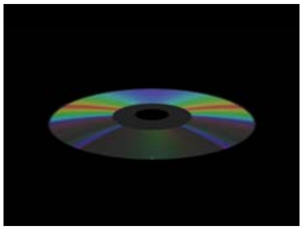
  Compare λ for an electron ($m_e = 9.1\times10^{-31}$ kg) traveling at speed of 1.0×10^7 m/s with that for a ball of mass 0.10 kg traveling at 35 m/s.

Chapter 6 Section 4

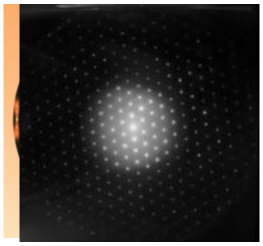
Diffraction Patterns

- ***Diffraction*** is the process when light is scattered from a regular array of points or lines.





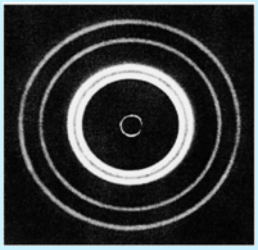
- When X-rays are directed onto a crystal of NaCl, a ***diffraction pattern*** (bright spots and dark areas) is produced. This can only be explained in terms of waves.



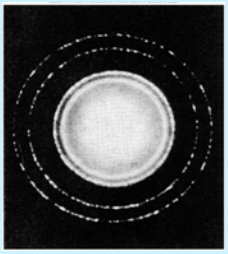
Chapter 6 Section 4

Diffraction of Electrons

- When a beam of electrons (instead of X-ray) was directed to a piece of aluminum, another diffraction pattern similar to that observed in the X-ray experiment was observed.
- Electrons, like X-ray, exhibit some wave-like properties.



X-ray diffraction pattern of Al foil

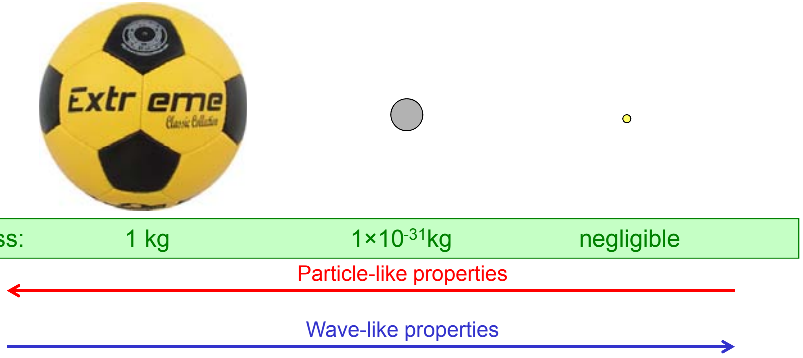


Electron diffraction pattern of Al foil

Chapter 6 Section 4

Particles or Waves?

- Energy is a form of matter and is not just waves. Energy and matter are not distinct.
- Matters and radiation exhibit both ***particle-like*** and ***wave-like*** properties. In other words matter is of dual nature.



Mass: 1 kg 1×10^{-31}kg negligible

Particle-like properties

Wave-like properties

Chapter 6 Section 5

Development of Quantum Mechanics

- The ***uncertainty principle*** by Heisenberg.

  It is *impossible* to determine *accurately* both the position, x, and the momentum, $p = m \times u$, (and accordingly speed) at a given time.

$$\boxed{\Delta x \cdot \Delta(m\upsilon) \ge \frac{h}{4\pi}}$$

- The uncertainty is very limited for large objects but has significance for very small objects like electrons.
- We can NOT know the exact motion for an electron around the nucleus, but we can define a space in which the electron can be found in an atom (***Probability***)

Chapter 6 Section 5

The Uncertainty Principle

- **According to Bohr model**, the electron orbits the nucleus of the hydrogen atom at definite paths "***orbits***".

  Bohr's model was applicable only for single-electron atoms.
- **According to Heisenberg uncertainty principle**, the electron can't orbit the nucleus of the hydrogen atom at definite paths. The uncertainty in the position of the electron is large. The best way to explain the motion of the electron is by considering the probability of finding the electron at different positions in the atom "***electron density***" or "***orbitals***"

Schrödinger Equation

$$\hat{H}\psi = E\psi$$

- ψ is the *wave* function that describes the electron's position in 3-D space "a complicated math function".
- $\hat{H}$ is the energy operator.
- E is the total energy which is the summation of the individual energies of each electron.
- ψ is also called an ***orbital***.
- ψ^2 is the probability of finding an electron in a given position of the atom.

Schrödinger equation describes the electron based on its ***wave-particle* behavior** (the quantum-mechanical electron)

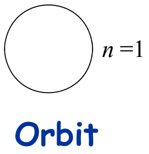
Electron Density (Probability Distribution)

- Schrödinger equation specifies the possible ***energy states*** that the electron in the hydrogen atom can occupy.
- Each one of these energy states is described by a specific wave function, ψ.
- The energy states and wave functions are characterized by a set of ***quantum numbers***.
- Bohr description involves ***orbits***, while quantum-mechanical description involves ***orbitals***.

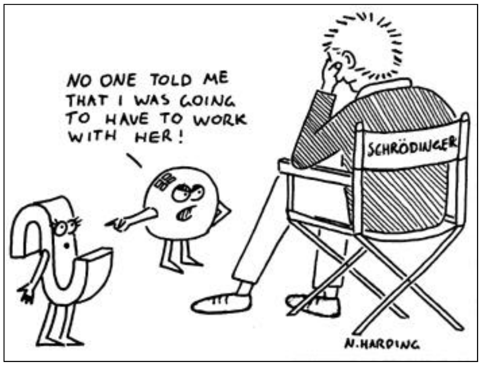
Chapter 6 Section 5

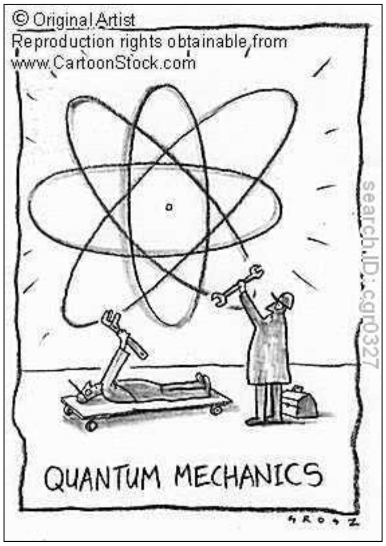
Quantum Mechanical Picture of the Atom vs. Bohr's Model

- In Bohr's model, the electron is assumed to have a *definite circular paths* (***orbits***). Thus, the electron is *always* found at these distances.



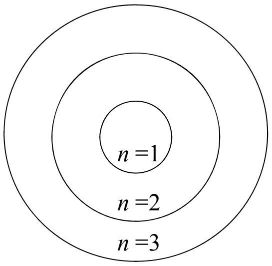
- In the (wave) quantum mechanical model, the electron motion is *not* exactly known, and we rather talk about the *probability* of finding the electron in a three-dimensional space around an atom (***orbital***).





Quantum Numbers

- In Bohr's model, only **one quantum number**, *n*, was necessary to describe the location of the electron in an atom.



- In quantum mechanics, **three quantum numbers** are needed to describe the distribution of the electron density in an atom. These quantum numbers are derived from the mathematical solution of Schrödinger equation.

Quantum Numbers

1. Principal quantum number (n):

- Has integer values: 1, 2, 3, … and sometimes called a "*shell*".
- The larger the value of n, the larger the **size** of the orbital is, and the more the electron to spend time far from the nucleus.
- The larger the value of n, the higher the **energy** of the electron.

2. Angular momentum quantum number (ℓ):

- ℓ has integer values from 0 to n-1 for each value of n.
- It describes the **shape** of the orbital, sometimes called a "*sub-shell*"

For n = 5 :

Value of ℓ	0	1	2	3	4
Letter Used	*s*	*p*	*d*	*f*	*g*

Chapter 6 Section 6

Quantum Numbers

3. Magnetic quantum number (m_ℓ):

- Has integer values from ℓ to $-\ell$ including $\ell = 0$.
- It is related to the **orientation** of the orbital in space with respect to the other orbitals.
- It indicates the *number of orbitals in a subshell* with a particular value of ℓ.

- To summarize:

$n = 1, 2, 3, \ldots$	(Energy and size)
$\ell = 0, 1, 2, \ldots, (n-1)$	(Shape)
$m_\ell = -\ell, (-\ell+1), \ldots, 0, \ldots, (\ell-1), +\ell$	(Orientation)

Chapter 6 Section 6

Quantum Numbers

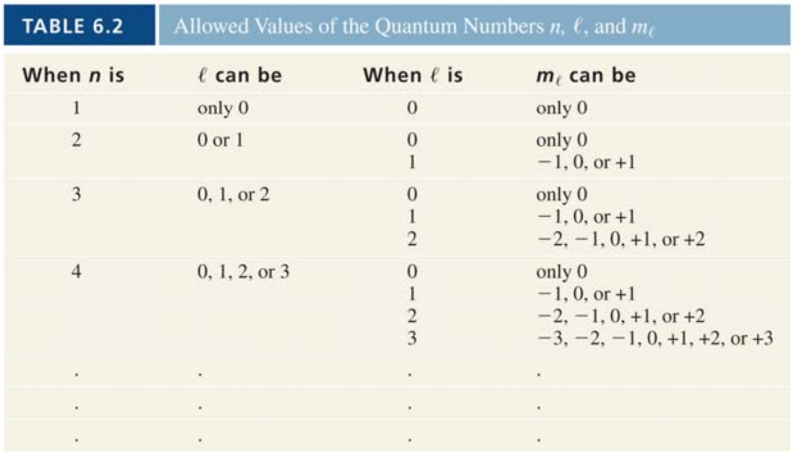


TABLE 6.2 Allowed Values of the Quantum Numbers n, ℓ, and m_ℓ

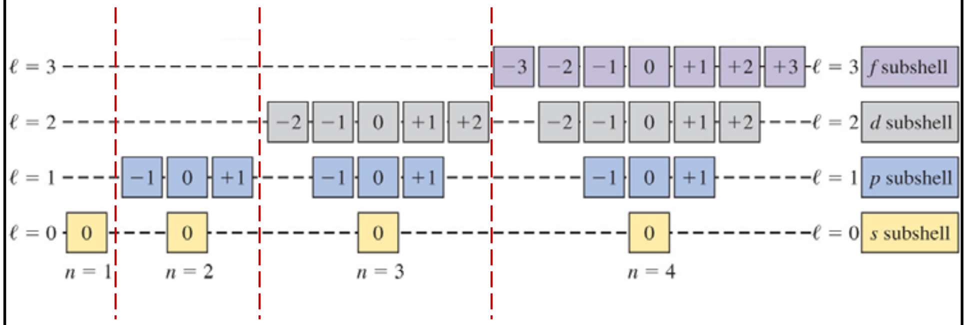
When n is	ℓ can be	When ℓ is	m_ℓ can be
1	only 0	0	only 0
2	0 or 1	0 1	only 0 −1, 0, or +1
3	0, 1, or 2	0 1 2	only 0 −1, 0, or +1 −2, −1, 0, +1, or +2
4	0, 1, 2, or 3	0 1 2 3	only 0 −1, 0, or +1 −2, −1, 0, +1, or +2 −3, −2, −1, 0, +1, +2, or +3
.	.	.	.
.	.	.	.
.	.	.	.

Example: For an orbital with $n = 2$ and $\ell = 1$, it symbolized as $2p$.

There are three $2p$ orbitals that have different orientations in the space.

Chapter 6 Section 6

Quantum Numbers



Example: For an orbital with $n = 3$ and $\ell = 0$, it symbolized as 3*s*.

There is only one 3*s* orbital.

Chapter 6 Section 6

Quantum Numbers

Exercise:

For $n = 4$, determine the number of allowed subshells and give the designation of each.

$n = 4$

$\ell =$ 0, 1, 2 and 3

4*s* 4*p* 4*d* 4*f*

Number of orbitals per subshell:

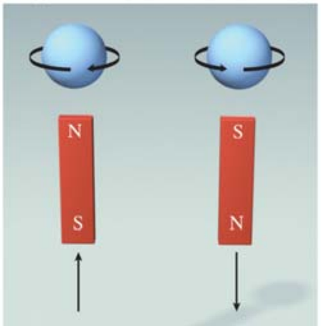
1 3 5 7

Exercise:

How many orbitals can the subshell 3*d* have?

Electron Spin Quantum Number (m_s)

- A spinning charged object generates a magnetic field. Thus, the electron behaves like a magnet.
- It was assumed that the electron has two possible spin directions, which can be described using a fourth quantum number (m_s) "*electron spin quantum number*"
  + ½ or – ½ .
- Any orbital is described by the three quantum numbers (n, ℓ, m_l). The fourth quantum number describes the spin of the electron.
- Each orbital can hold maximum of two electrons that must have opposite spins. The electrons are said to be **paired**.



Exercise

Which of the following sets of quantum numbers are not allowed?

(a) $n = 3$, $\boxed{\ell = -2}$, $m_\ell = 2$.

(b) $\boxed{n = 0}$, $\ell = 0$, $m_\ell = 0$.

(c) $n = 4$, $\ell = 1$, $m_\ell = 1$, $m_s = +1/2$ ***OK***

(d) $n = 3$, $\ell = 1$, $\boxed{m_\ell = 2}$, $m_s = -1/2$

Chapter 6 Section 6

Exercise

Give the maximum number of electrons in an atom that can have these quantum numbers:

(a) $n = 4$. (b) $n = 5$ and $m_\ell = +1$ (c) $n = 5$ and $m_s = +1/2$.

(d) $n = 3$ and $\ell = 2$

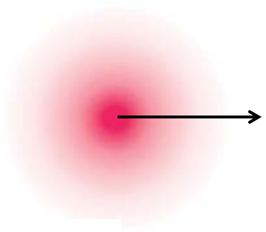
Chapter 6 Section 7

Atomic Orbitals

Probability of finding an e$^-$ around the nucleus (ψ^2) is often called ***orbital***.

- Taking the **1*s*** orbital as an example.

Spherical 3D

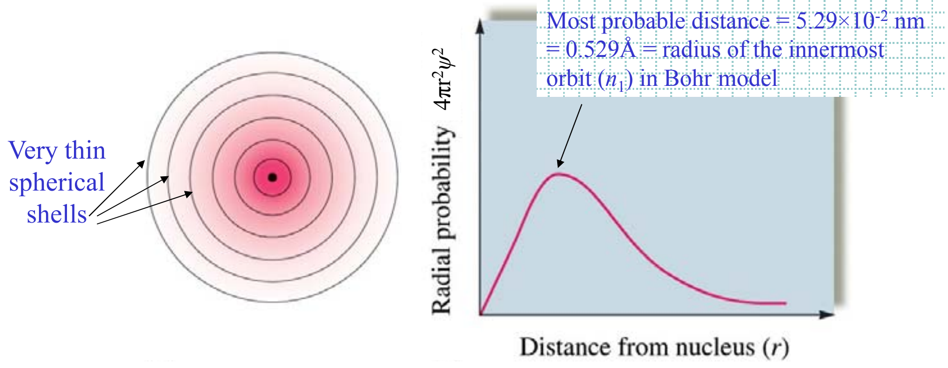


The more times the electron visits a particular point, more electron density (more probability) builds up at that particular point and the darker the negative becomes. Thus, the electron is more probably to be found at the darker areas.

Chapter 6 Section 7

Atomic Orbitals

- *Radial probability* distribution for the **1*s*** orbital



Most probable distance = 5.29×10^{-2} nm = 0.529Å = radius of the innermost orbit (n_1) in Bohr model

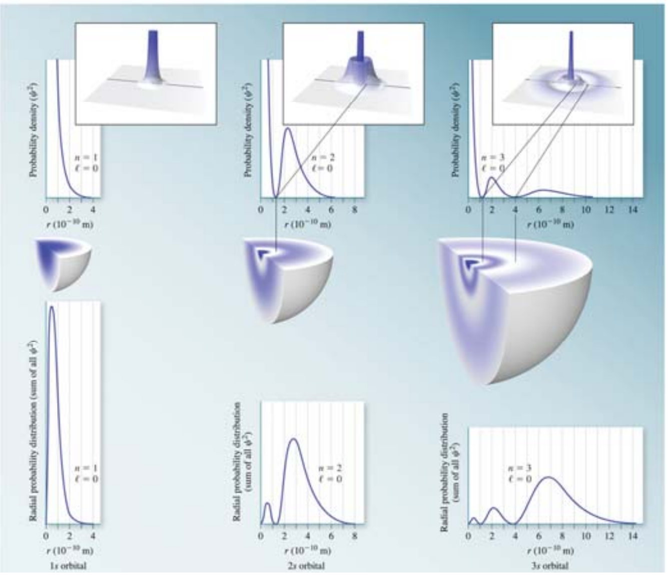
Very thin spherical shells

It is a factor of both the probability density and the area of the spherical shell at a particular distance form the nucleus.

Chapter 6 Section 7

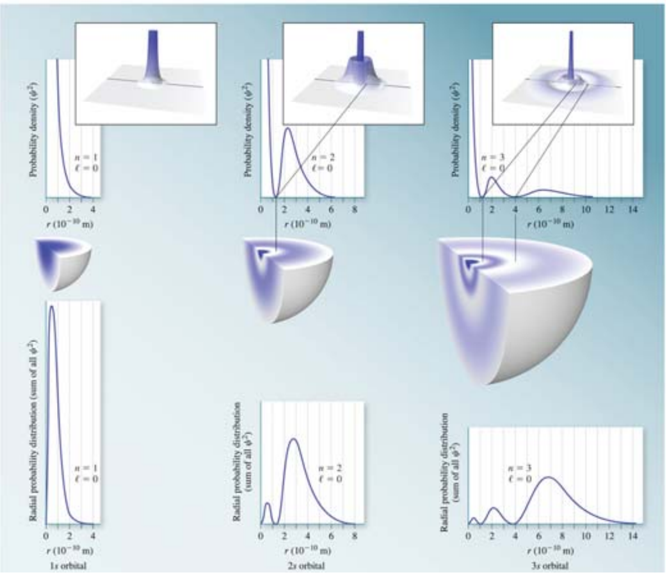
Orbital Shapes, *s* Orbitals (ℓ = 0)

- We are looking here for the angular momentum quantum number (ℓ).
- ℓ = 0 (spherical).
- All *s* orbitals are similar in shape but different in energy and size.
- Size of orbital is proportional to *n*.



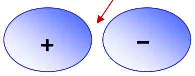
Orbital Shapes, *s* Orbitals ($\ell = 0$)

- Zero probability region is called a *node*.
  # of nodes = $n - 1$.
- The orbital size or boundary is 90% probability (by definition).

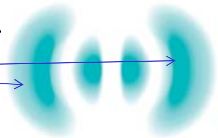


Orbital Shapes, *p* Orbital ($\ell = 1$)

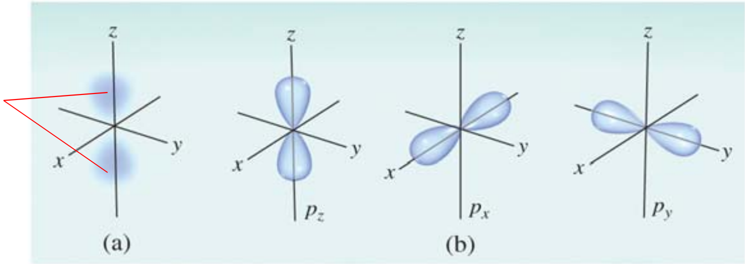
The node here is centered at the nucleus



- No *p* orbitals at $n = 1$.
- Two "lobes" separated by a node.
- p_x, p_y and p_z orbitals are identical in energy.
- The shape of 3*p* orbitals is similar but of a larger size.



Lobes



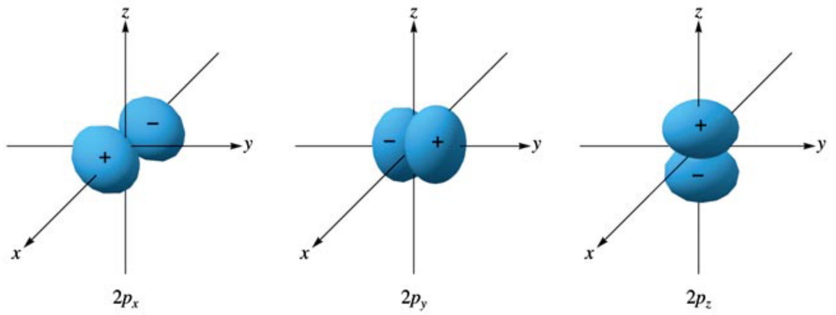
Chapter 6 Section 7

Orbital Shapes, *p* Orbital ($\ell = 0$)

$n = 2, 3, 4, \ldots$

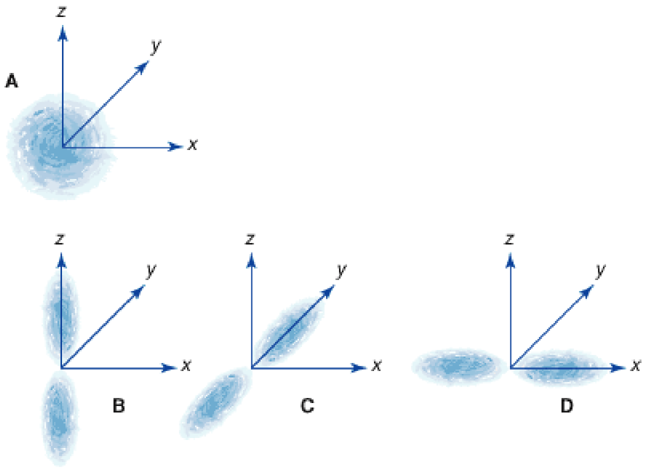
$\ell = 1$ (*p* orbitals)

$m_\ell = -1$ 0 +1



Chapter 6 Section 7

Orbital Shapes, *s* and *p* Orbitals

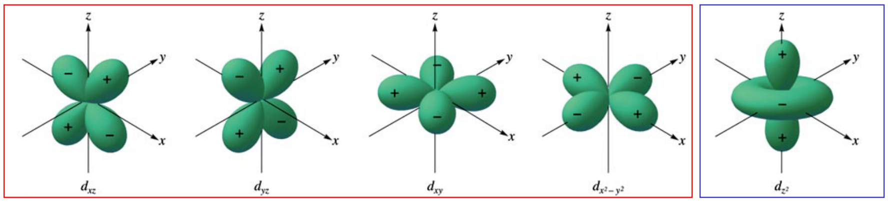


Chapter 6 Section 7

Orbital Shapes, *d* Orbital ($\ell = 2$)

- Start at $n = 3$ (or $\ell = 2$ “five *d*-orbitals”).
- The five *d*-orbitals are identical in energy.
- *d* orbitals have two different fundamental shapes.
- For $n > 3$, *d* orbitals look like the 3*d* ones but with larger lobes.

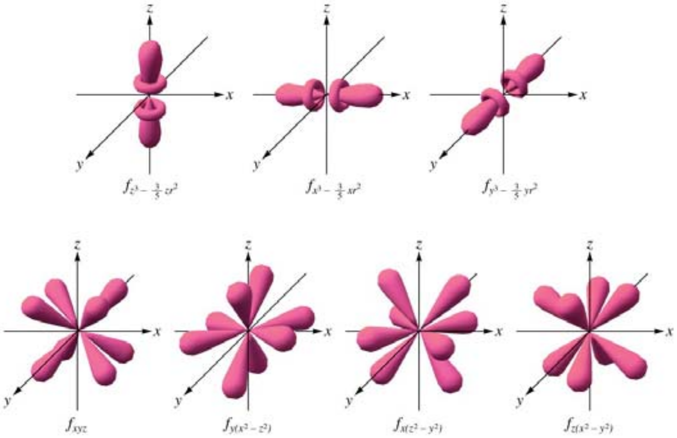
$m_\ell =$ -2 -1 0 +1 +2



Chapter 6 Section 7

Orbital Shapes, *f* Orbitals ($\ell = 3$)

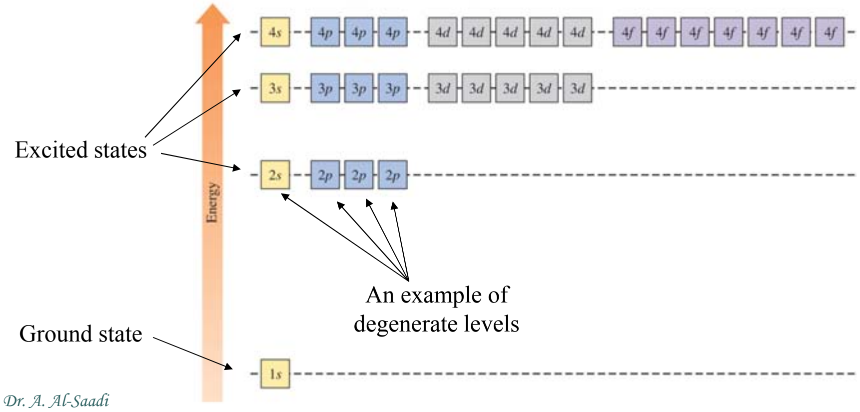
- Start at $n = 4$ (or $\ell = 3$ “seven *f*-orbitals”).



Chapter 6 Section 7

Orbital Energies in Hydrogen Atom

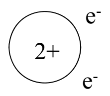
- They are determined by the value of *n*.
- In the case of ***hydrogen atom*** or ***hydrogen-like atoms***, we call orbitals of the same *n* (with same energies) ***degenerate***.

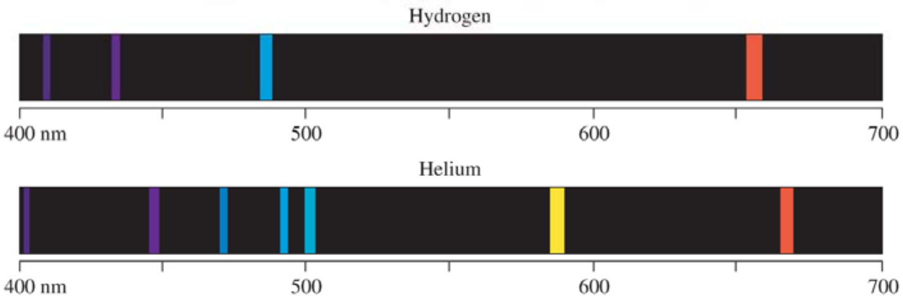


Chapter 6 Section 8

Orbital Energies in Many-Electron Atom

- Why is the He emission spectrum is different than the H emission spectrum?
- There is a splitting of energy levels due to $e^- - e^-$ repulsion.

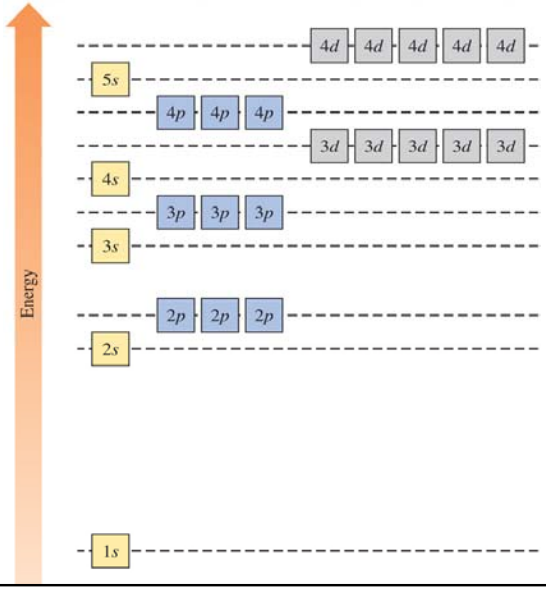




Chapter 6 Section 8

Orbital Energies in Many-Electron Atom

- In many-electron systems, the orbitals split.
- In this case, the energies of orbitals depend not only on the quantum number *n*, but also ℓ.
- For a given *n*, the energy of the orbitals increases with the increase of the value of ℓ.



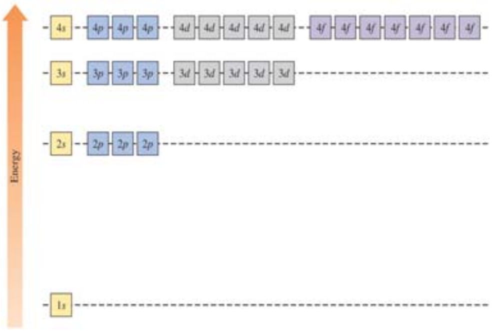
Chapter 6 Section 8

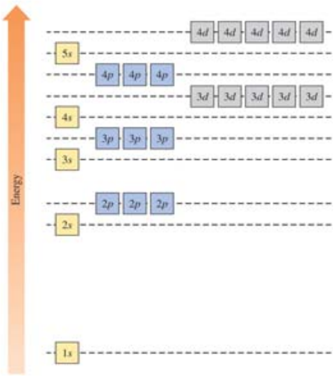
Orbital Energies in Many-Electron Atom

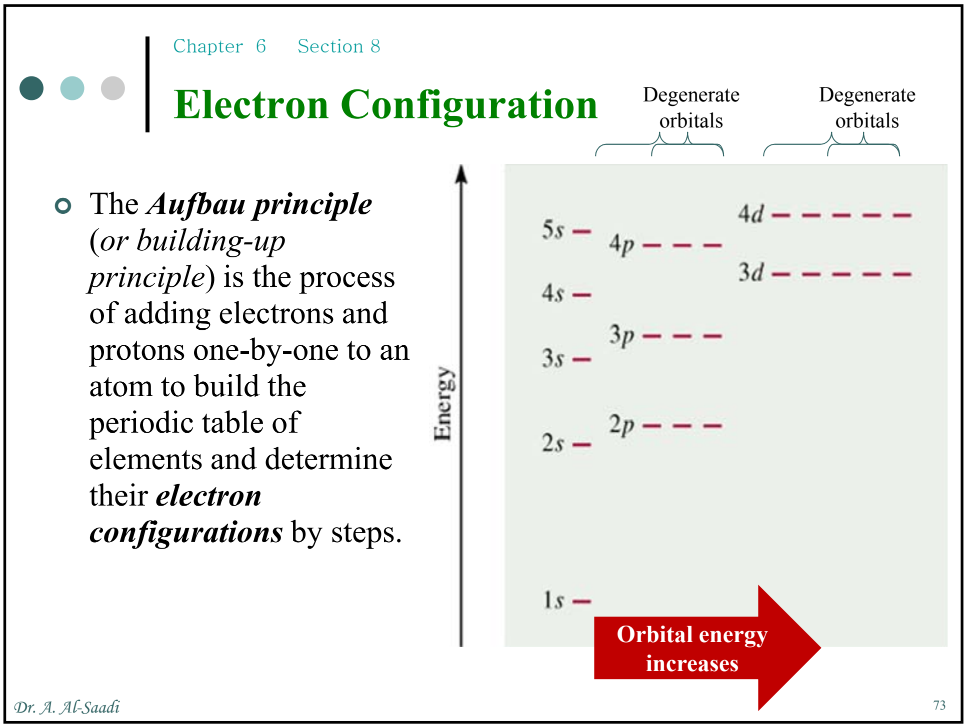
Hydrogen-like atoms **Many-electron atoms**

Both have the same general shapes

$E_{ns} = E_{np} = E_{nd} = E_{nf}$ $E_{ns} < E_{np} < E_{nd} < E_{nf}$

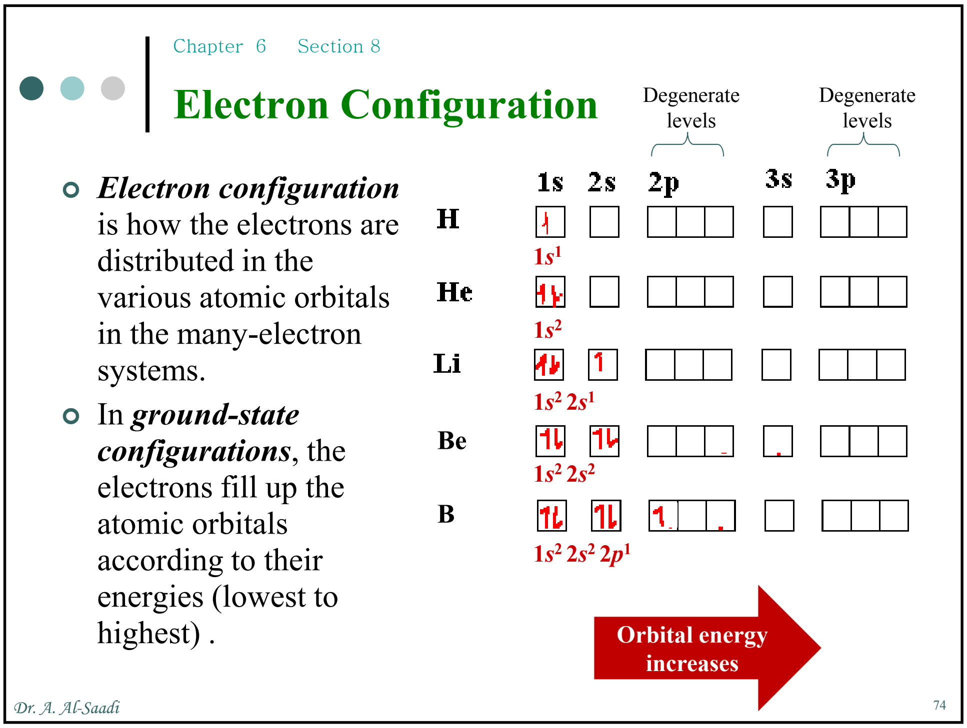






Electron Configuration

- The ***Aufbau principle*** (*or building-up principle*) is the process of adding electrons and protons one-by-one to an atom to build the periodic table of elements and determine their ***electron configurations*** by steps.



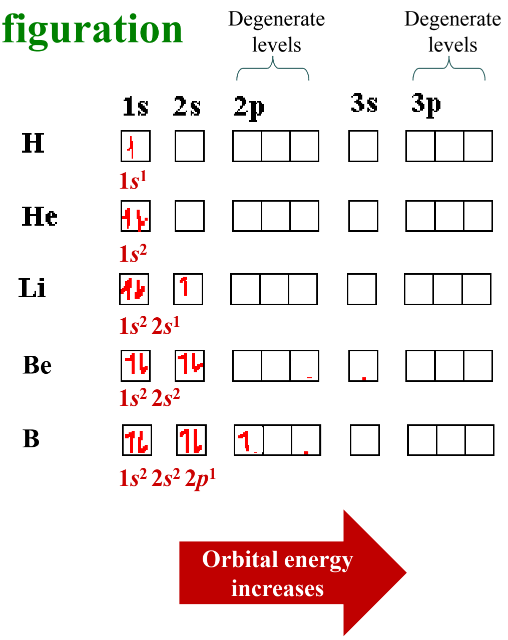
Electron Configuration

- ***Electron configuration*** is how the electrons are distributed in the various atomic orbitals in the many-electron systems.
- In ***ground-state configurations***, the electrons fill up the atomic orbitals according to their energies (lowest to highest) .

	1s	2s	2p	3s	3p
H	↑	☐	☐☐☐	☐	☐☐☐
	$1s^1$				
He	↑↓	☐	☐☐☐	☐	☐☐☐
	$1s^2$				
Li	↑↓	↑	☐☐☐	☐	☐☐☐
	$1s^2\ 2s^1$				
Be	↑↓	↑↓	☐☐☐	☐	☐☐☐
	$1s^2\ 2s^2$				
B	↑↓	↑↓	↑☐☐	☐	☐☐☐
	$1s^2\ 2s^2\ 2p^1$				

Electron Configuration

- The ***Pauli exclusion principle*** states that no two electrons in an atom can have the same four quantum numbers.
- A maximum of two electrons may occupy an atomic orbitals, with opposite spins.
- Next is the C atom.



Hund's Rule

- The most stable configuration of electrons in degenerate atomic orbitals is the one having the number of electrons with the same spin be maximized.
- This requires putting the same-spin electrons in separate degenerate orbitals before paring them with electrons having the opposite spin.

Repulsive electrons will occupy separate degenerate orbitals.

Ne: $1s^2 2s^2 2p^6$

Na: $1s^2 2s^2 2p^6\ 3s^1$

$[\text{Ne}]3s^1$

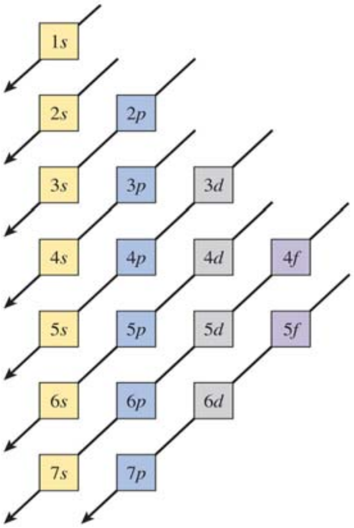
an outermost electron

noble gas core

Chapter 6 Section 8

Rules of Writing Electron Configurations

1. Electrons reside in orbitals of the lowest possible energy.
2. Maximum of two electrons per orbital. (Pauli Exclusion Principle)
3. Electrons do not pair in degenerate orbitals if an empty orbital is available. (Hund's Rule)
4. Orbitals fill in order of increasing energy.



Chapter 6 Section 9

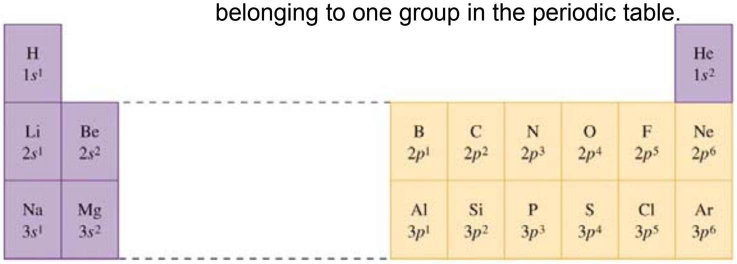
Electron Configurations and the Periodic Table

Na: $1s^22s^22p^6\,3s^1$
[Ne] $3s^1$
Mg: [Ne] $3s^2$
Al: [Ne] $3s^2\,3p^1$

Ar: [Ne] $3s^2\,3p^6$

Noble gas core Inner electrons	Electrons in the outermost level
Core electrons	***Valence electrons***

The elements in the same group have the same *valence electron* configuration. This explains the similar chemical properties shown by elements belonging to one group in the periodic table.



H $1s^1$							He $1s^2$
Li $2s^1$	Be $2s^2$	B $2p^1$	C $2p^2$	N $2p^3$	O $2p^4$	F $2p^5$	Ne $2p^6$
Na $3s^1$	Mg $3s^2$	Al $3p^1$	Si $3p^2$	P $3p^3$	S $3p^4$	Cl $3p^5$	Ar $3p^6$

Chapter 6 Section 9

Electron Configurations of 3*d* Transition Metals

The **(*n*+1)*s*** orbitals always fill before the **(*n*)*d*** orbitals

K: $1s^22s^22p^6\,3s^2\,3p^6\,4s^1$ (NOT $3d^1$)
Ca: $1s^22s^22p^6\,3s^2\,3p^6\,4s^2$ (NOT $3d^2$)

K: [Ar] $4s^1$
Ca: [Ar] $4s^2$

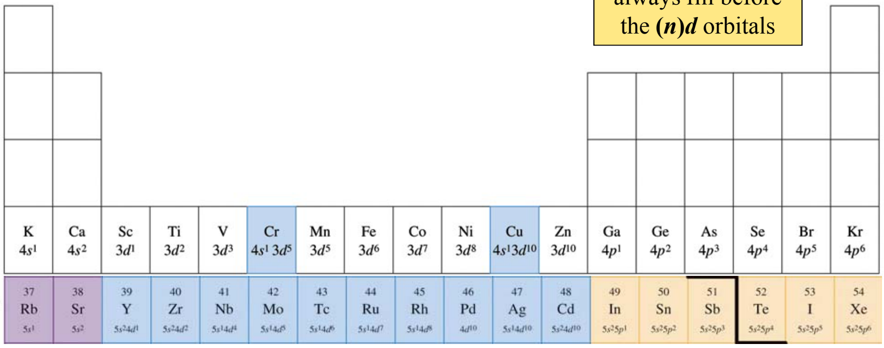
Transition metals

Sc: [Ar] $4s^23d^1$
Ti: [Ar] $4s^23d^2$
V: [Ar] $4s^23d^3$
Cr: [Ar] $4s^13d^5$ ← Exception (NOT [Ar] $4s^23d^4$)
Mn: [Ar] $4s^23d^5$
Fe: [Ar] $4s^23d^6$
Co: [Ar] $4s^23d^7$
Ni: [Ar] $4s^23d^8$
Cu: [Ar] $4s^13d^{10}$ ← Exception (NOT [Ar] $4s^23d^9$)
Zn: [Ar] $4s^23d^{10}$

Chapter 6 Section 9

Electron Configurations of 4*d* Transition Metals

The **(*n*+1)*s*** orbitals always fill before the **(*n*)*d*** orbitals



K $4s^1$	Ca $4s^2$	Sc $3d^1$	Ti $3d^2$	V $3d^3$	Cr $4s^1\,3d^5$	Mn $3d^5$	Fe $3d^6$	Co $3d^7$	Ni $3d^8$	Cu $4s^13d^{10}$	Zn $3d^{10}$	Ga $4p^1$	Ge $4p^2$	As $4p^3$	Se $4p^4$	Br $4p^5$	Kr $4p^6$
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 $5s^14d^6$	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 $5s^25p^6$

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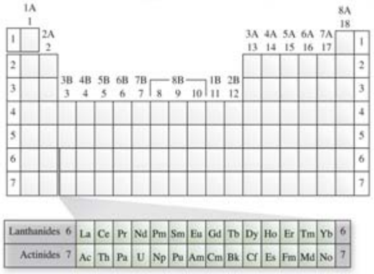
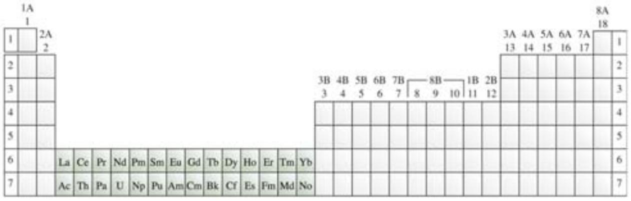
Electron Configurations of Lanthanides and Actinides

La: [Xe] $6s^2 5d^1$

Ac: [Rn] $7s^2 6d^1$

- ***Lanthanides*** and ***actinides*** have their ***4f*** and ***5f*** orbitals being filled, respectively.
- The energies of ***4f*** and ***5d*** orbitals are very close. The same thing is said for the energies of ***5f*** and ***6d*** orbitals.





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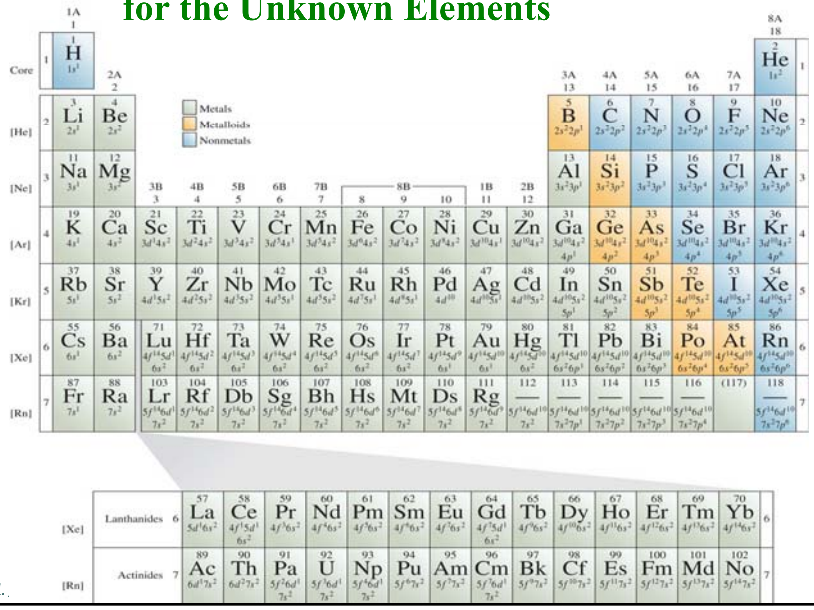
Ground-State Electron Configurations for the Unknown Elements



Dr. A.

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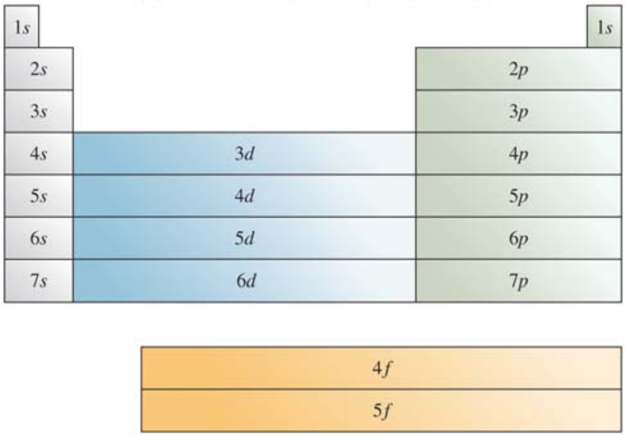
Electron Configuration and Periodic Table

From knowing the blocks of the periodic table as classified based on the types of subshells, one should be able to give the correct electron configurations.



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Exercise

Give the electron configurations for

- sulfur (S),
- cadmium (Cd),
- hafnium (Hf), and
- radium (Ra).