Chapter 6

Quantum Theory and the Electronic Structure of Atoms

Topics

- The nature of light
- Quantum theory
- Bohr's theory of the hydrogen atom
- Wave properties of matter
- Quantum mechanics
- Quantum numbers
- Atomic orbitals
- Electron configuration
- Electron configuration and the periodic Table

6.1 The Nature of Light

- electromagnetic radiation:
  - form of energy that acts as a wave as it travels
  - includes: X rays, Ultraviolet, visible light, infrared light, microwaves, and radio waves
  - It travels in waves at a speed of 2.9979×10^8 m/s in a vacuum
- All forms of EMR are combined to form electromagnetic spectrum

Low Energy

Electromagnetic Spectrum

High Energy

The whole range of frequencies is called “Spectrum”

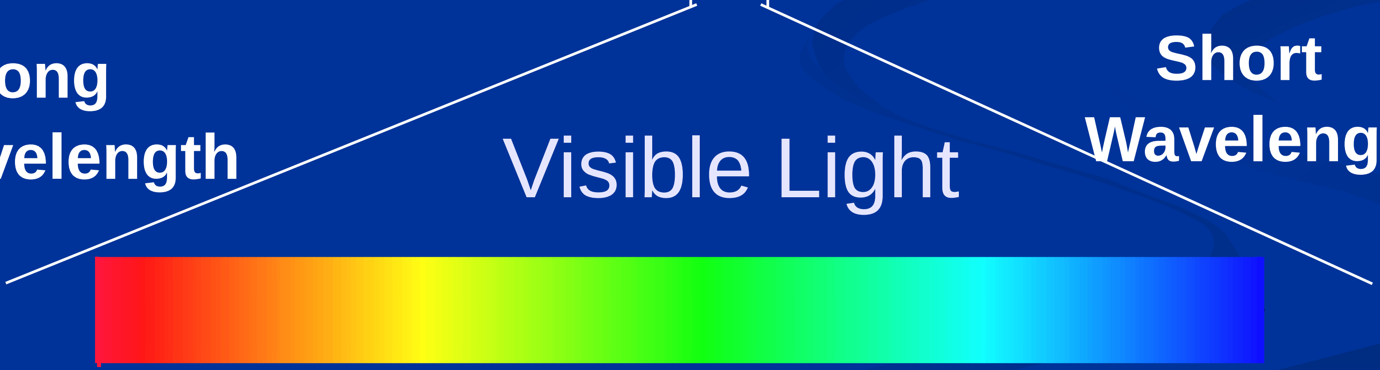
Radio waves	Micro waves	Infrared		Ultra-violet	X-Rays	Gamma Rays

Low Frequency

High Frequency

Long Wavelength

Short Wavelength

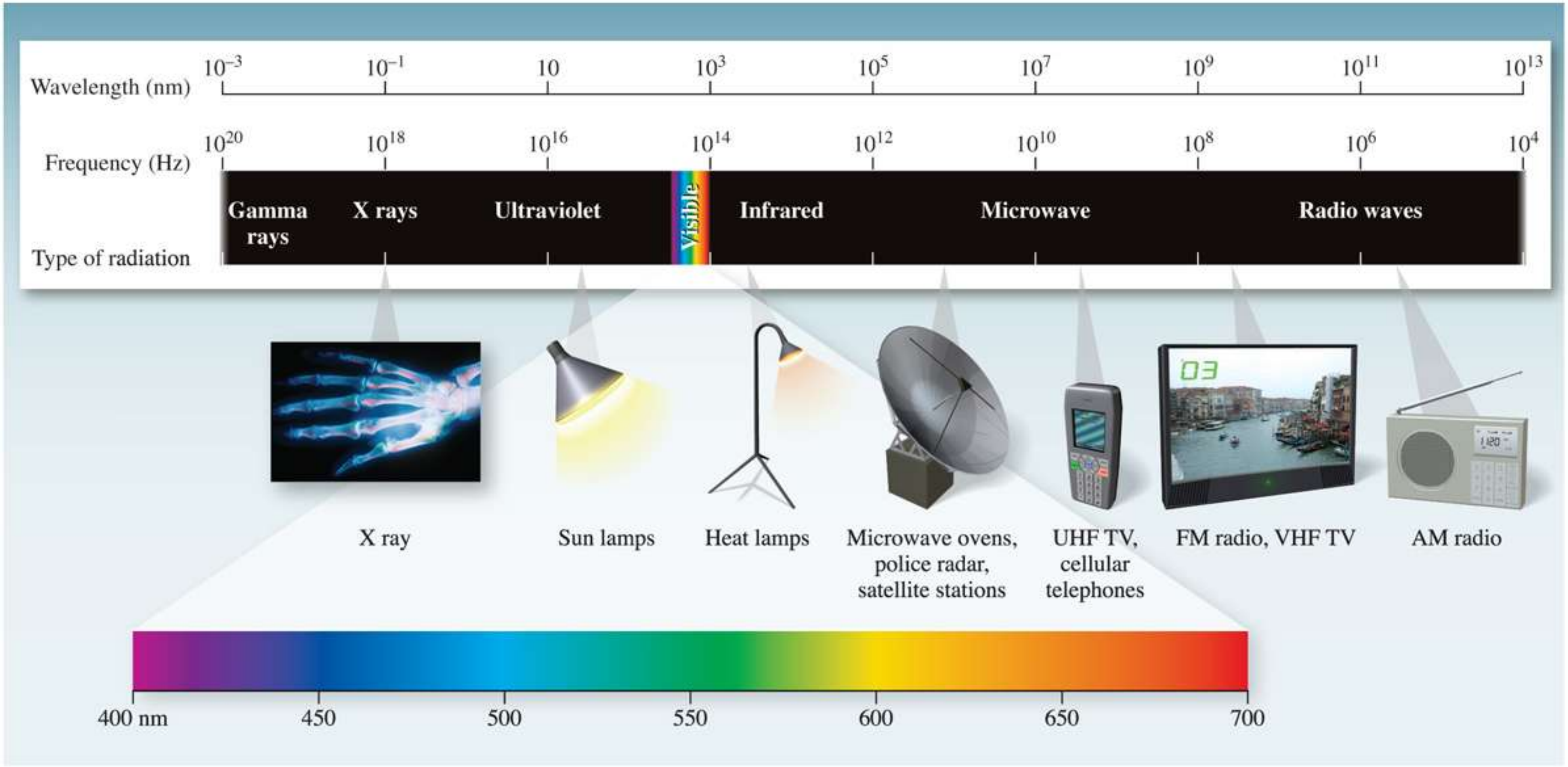


Visible Light

R O Y G B I V”

Visible light accounts for only a small part of the spectrum

Electromagnetic Spectrum



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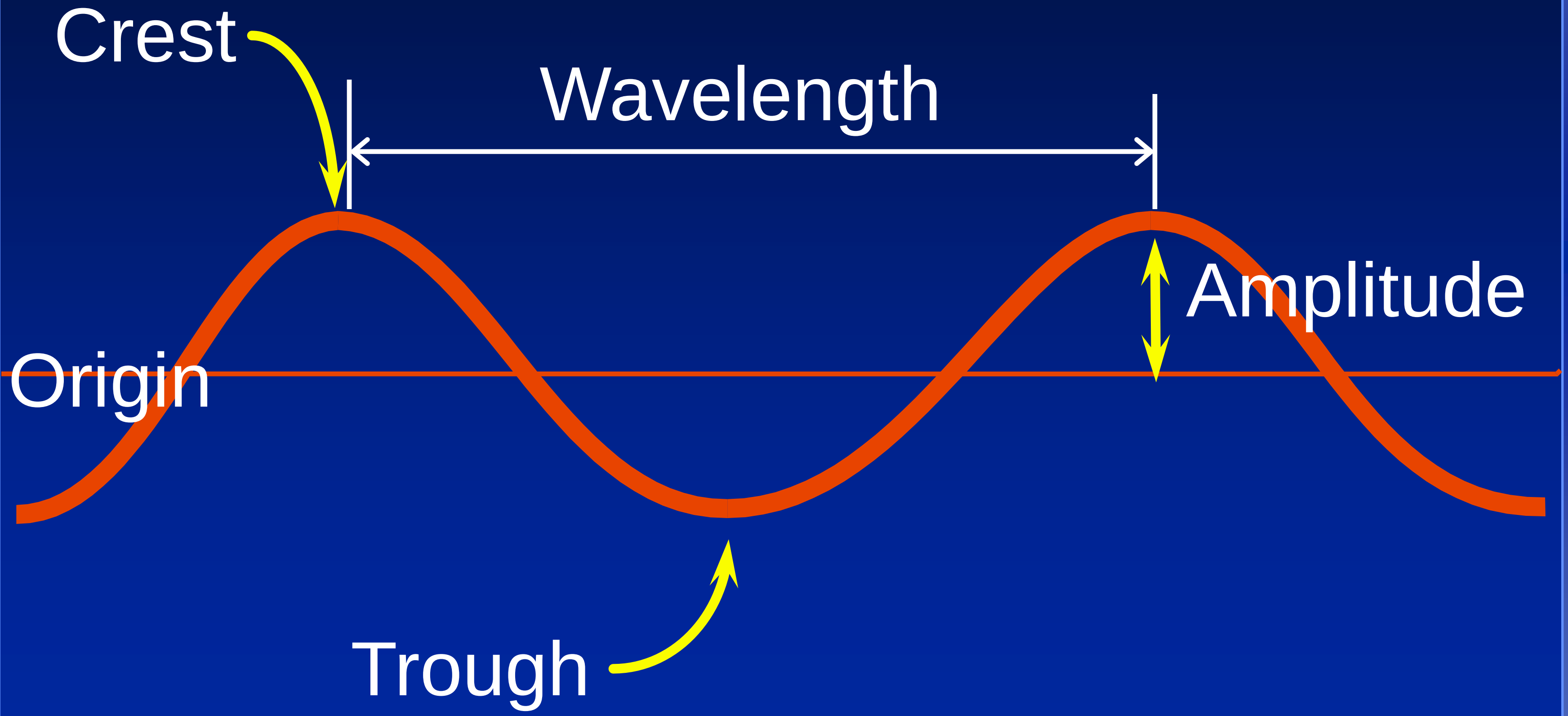
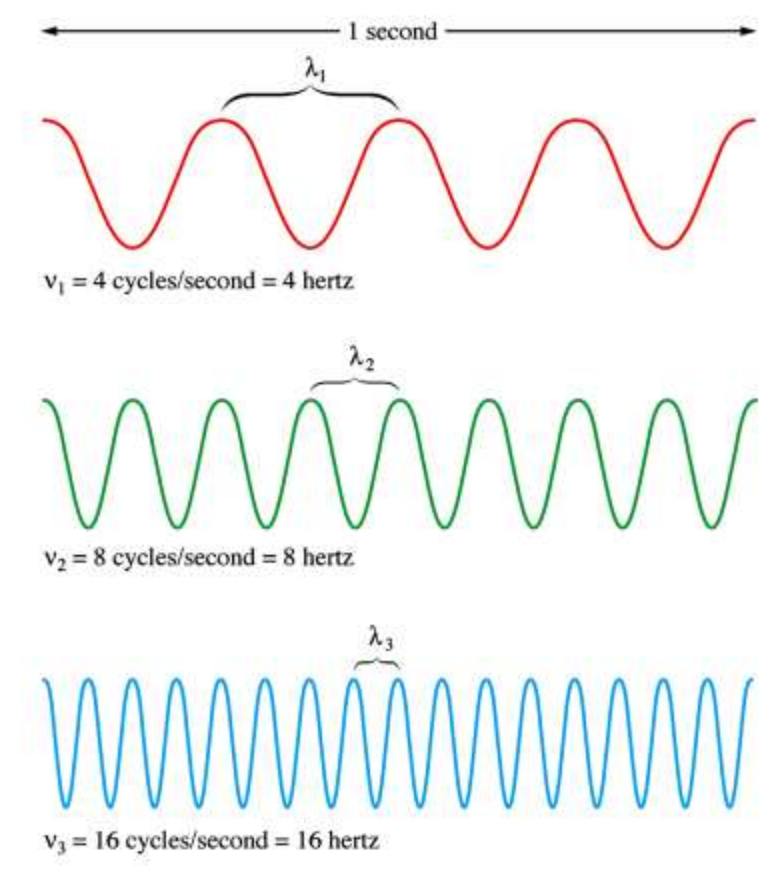
Wave Characteristics



- Wavelength
  - λ = Greek letter lambda
  - distance between points on adjacent waves (consecutive peaks or troughs)
  - Units used are in nm (10^9nm = 1m)
- Frequency
  - υ = Greek letter nu
  - number of wave cycles that passes a point in a second. 10^8 cycles/s= 10^8 s^{-1}
  - =10^8 Hertz = 10^8 Hz
  - in 1/second (Hertz = Hz)
- Amplitude

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

Electromagnetic radiation propagates through space as a wave moving at the speed of light.



Equation:

$$\boxed{c = \lambda \upsilon}$$

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

c = speed of light, a constant (2.998 x 10^8 m/s)

λ (lambda) = wavelength, in meters

ν (nu) = frequency, in units of hertz (hz or sec^{-1})

Wave Calculation

The wavelength of a laser pointer is reported to be 663 nm. What is the frequency of this light?

$$\upsilon = \frac{c}{\lambda}$$

$$\lambda = 663\ \text{nm} \times \frac{10^{-9}\ \text{m}}{\text{nm}} = 6.63 \times 10^{-7}\ \text{m}$$

$$\upsilon = \frac{3.00 \times 10^{8}\ \text{m/s}}{6.63 \times 10^{-7}\ \text{m}} = 4.52 \times 10^{14}\ \text{s}^{-1}$$

6.2 Quantum Theory

- According to the old views, matter could absorb or emit any quantity (frequency) of energy.
- **Max Planck** studied the radiation emitted by solid bodies heated to incandescence.
- **Max Planck** found that the cooling of hot objects couldn’t be explained by viewing energy as a wave.
- **Max Planck** postulated that energy can be gained (absorbed) or lost (emitted in discrete quantities

Nature of Matter

Mack's Planck suggested that an object absorbs or emits energy in the form of small packets of energy called quanta. That is the energy is quantized

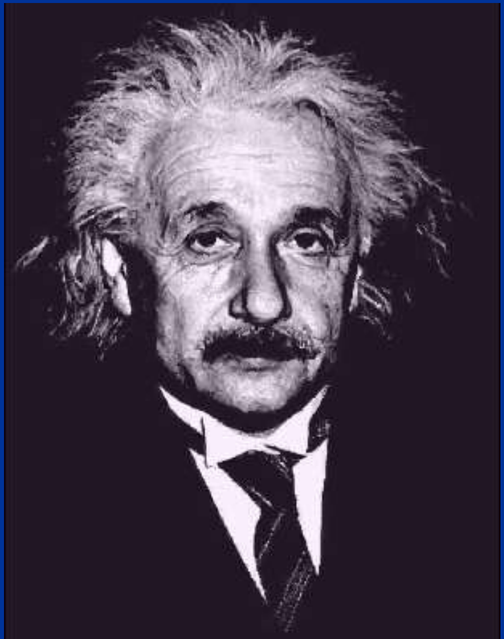
- Quantum- the minimum amount of energy that can be gained or lost by an atom (energy in each packet

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

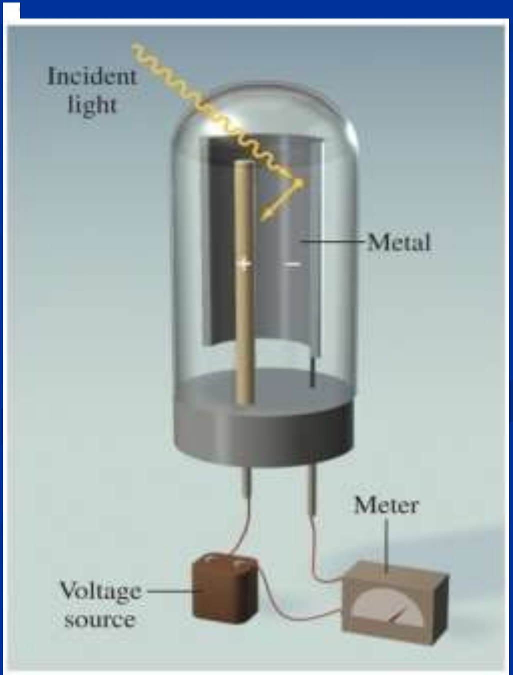
- h =Planck's constant= 6.626x10^{-34} J.s
- Thus energy seems to have particulate properties

Photoelectric Effect

- Albert Einstein used Planck's theory to explain photoelectric effect
- Electrons ejected from a metal's surface when exposed to light of certain frequency
- Einstein suggested that a beam of light is really a stream of particles
- Einstein called the particles of light photons (**packets of light energy**) and deduced that



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



- Only light with a frequency of photons such that $h\nu$ equals the energy that binds the electrons in the metal is sufficiently energetic to eject electrons.
- If light of higher frequency (enough to break the electrons free) is used, electrons will be ejected and will leave the metal with additional kinetic energy.

  $h\nu = KE + W$ (the binding energy of electrons in the metal)
- Light of at least the threshold frequency and of greater *intensity* will eject *more* electrons.

Calculate the energy (in joules) of a photon with a wavelength of 700.0 nm

$$\lambda = 700.0\ \text{nm} \times \frac{10^{-9}\ \text{m}}{\text{nm}} = 7.00 \times 10^{-7}\ \text{m}$$

$$\upsilon = \frac{c}{\lambda} = \frac{3.00 \times 10^{8}\ \text{m/s}}{7.00 \times 10^{-7}\ \text{m}} = 4.29 \times 10^{14}\ \text{s}^{-1}$$

$$E = h\upsilon = (6.63 \times 10^{-34}\ \text{J} \cdot \text{s})(4.29 \times 10^{14}\ \text{s}^{-1})$$

$$E = 2.84 \times 10^{-19}\ \text{J}$$

Example

Calculate the wavelength (in nm) of light with energy 7.83x 10^{-19} J per photon. In what region of the electromagnetic radiation does this light fall?

$$\upsilon = \frac{7.83\times 10^{-19}\,\mathrm{J}}{6.63\times 10^{-34}\,\mathrm{J\cdot s}} = 1.18\times 10^{15}\,\mathrm{s}^{-1}$$

$$\lambda = \frac{3.00\times 10^{8}\,\mathrm{m\cdot s^{-1}}}{1.18\times 10^{15}\,\mathrm{s}^{-1}} = 2.53\times 10^{-7}\,\mathrm{m} \quad \text{or } 253\ \mathrm{nm}$$

Ultraviolet region

Light possesses wave and particle properties

- Dilemma caused by Einestien’s theory - is light a wave or particle?
- Conclusion: Light must have particle characteristics as well as wave characteristics
- This concept is found to be applicable for all matter.

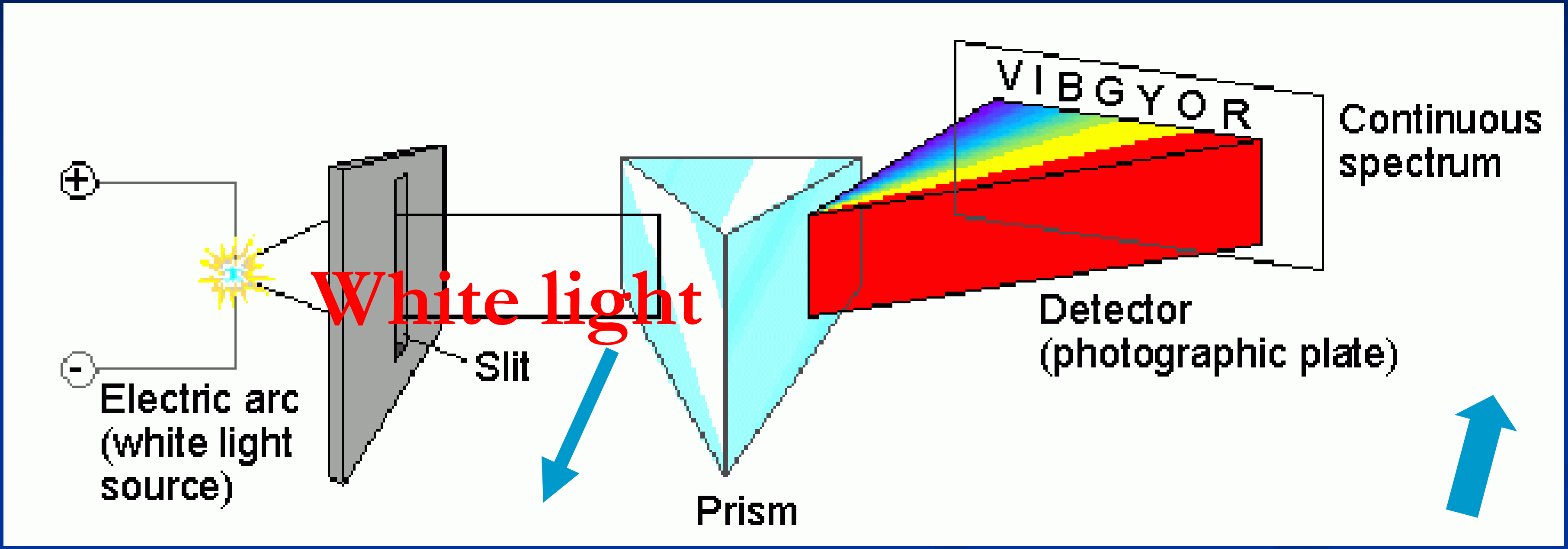
6.3 Bohr's Theory of the Hydrogen Atom

- Planck's theory along with Einstein's ideas not only explained the photoelectric effect, but also made it possible for scientists to unravel the idea of atomic line spectra

Emission Spectrum

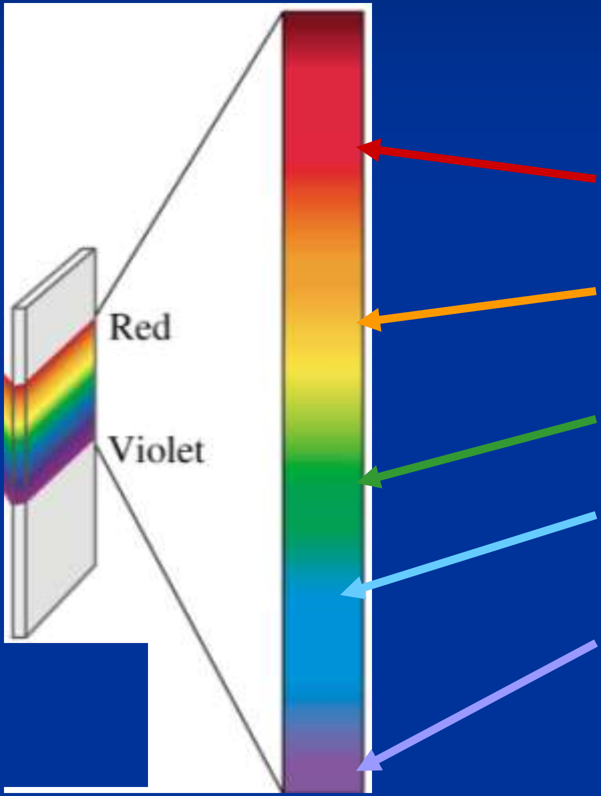
- Main experiments led to the information related to atom:
  - Thompson discovery of electron
  - Rutherford discovery of nucleus
  - Study of emission of spectrum
- The emission spectrum of a substance can bee seen by energizing a sample of material with either a thermal energy or other some form of energy
- The glow of a red –hot object is the emitted radiation in the visible region
- The emission spectrum of the sun or the heated solid is continuous that is all wavelengths of visible light are present in each spectrum

Spectroscopic analysis of the visible spectrum



- When sunlight is dispersed by rain drops the rainbow is Produced; that is a **continuous** spectrum is produced.
- continuous spectrum contains all colors; that is all wavelengths of the visible light

The Continuous Spectrum



$\lambda \sim 650$ nm

$\lambda \sim 575$ nm

$\lambda \sim 500$ nm

$\lambda \sim 480$ nm

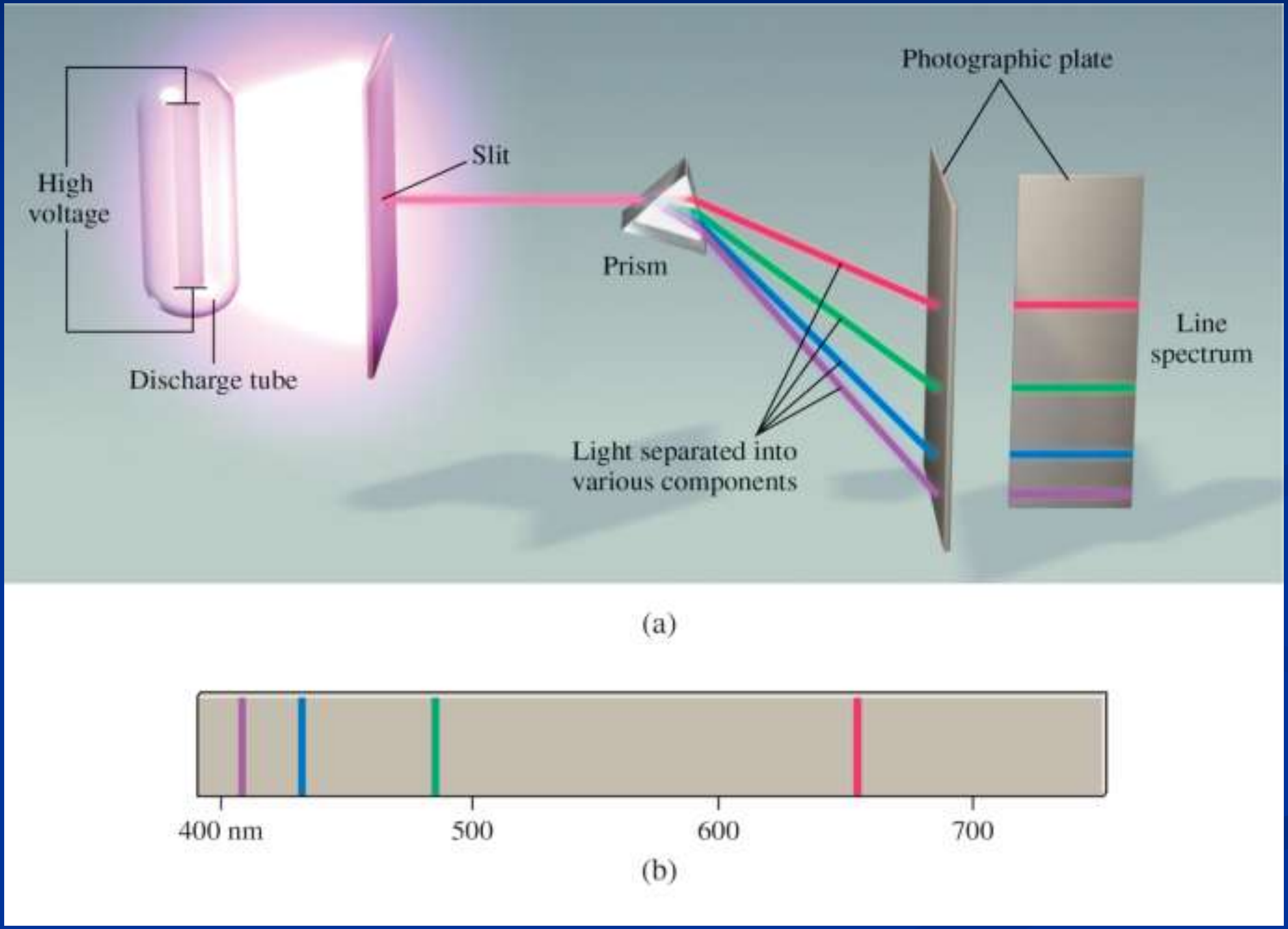
$\lambda \sim 450$ nm

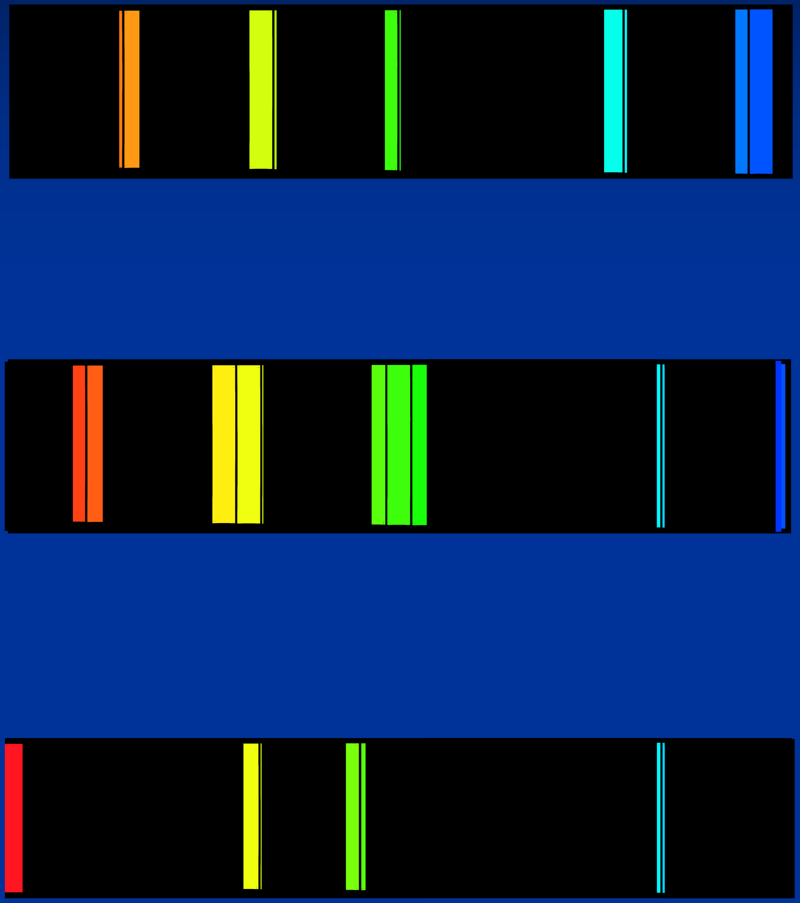
The different colors of light correspond to different wavelengths and frequencies

Atomic Line Spectra

- ***Line spectra***: emission of light only at specific wavelengths
- **Every element has a unique emission spectrum**
- **Often referred to as "fingerprints" of the element**

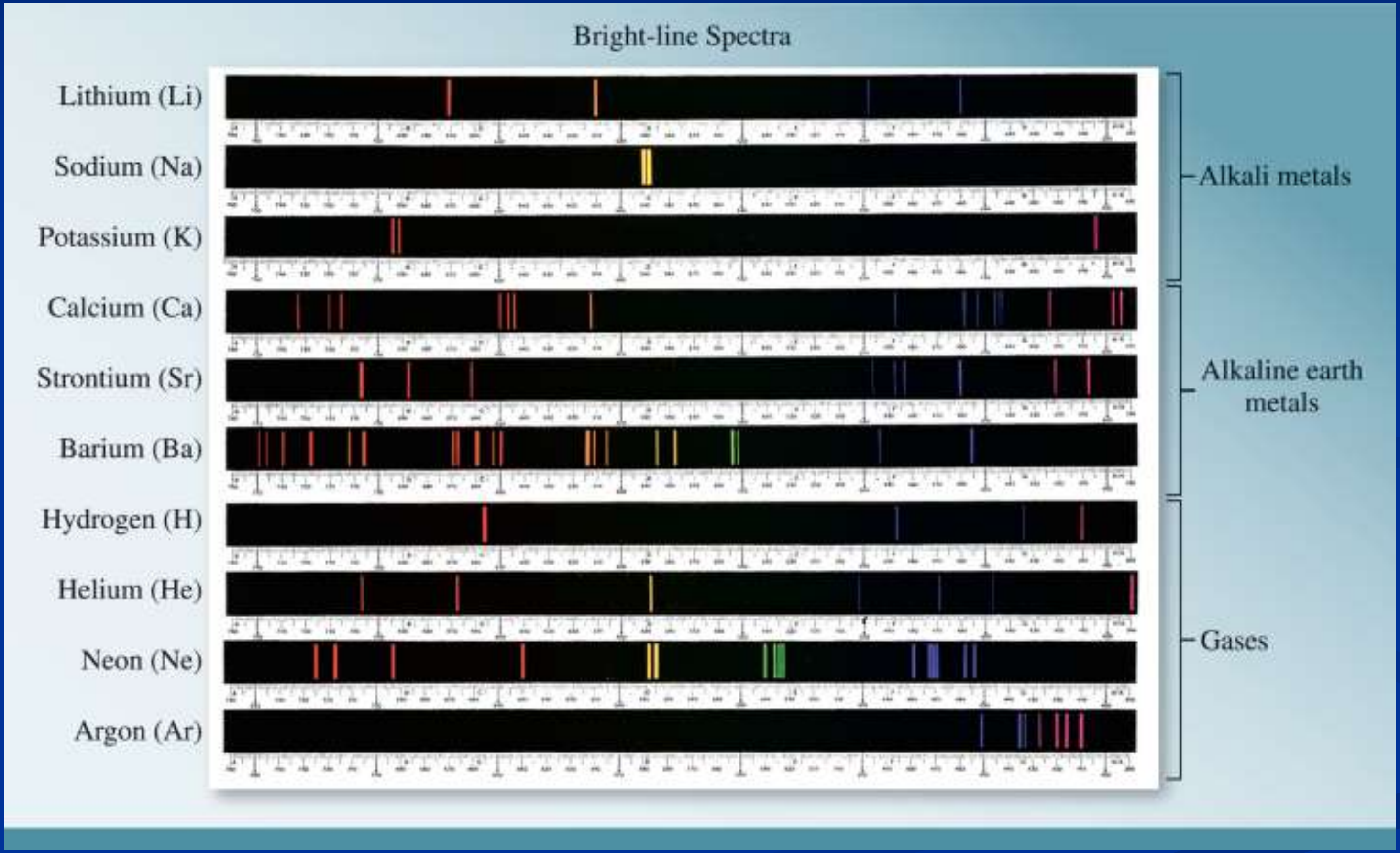
Atomic Line Spectra





- Line spectrum
- Unique to each element, like fingerprints!
- Very useful for identifying elements

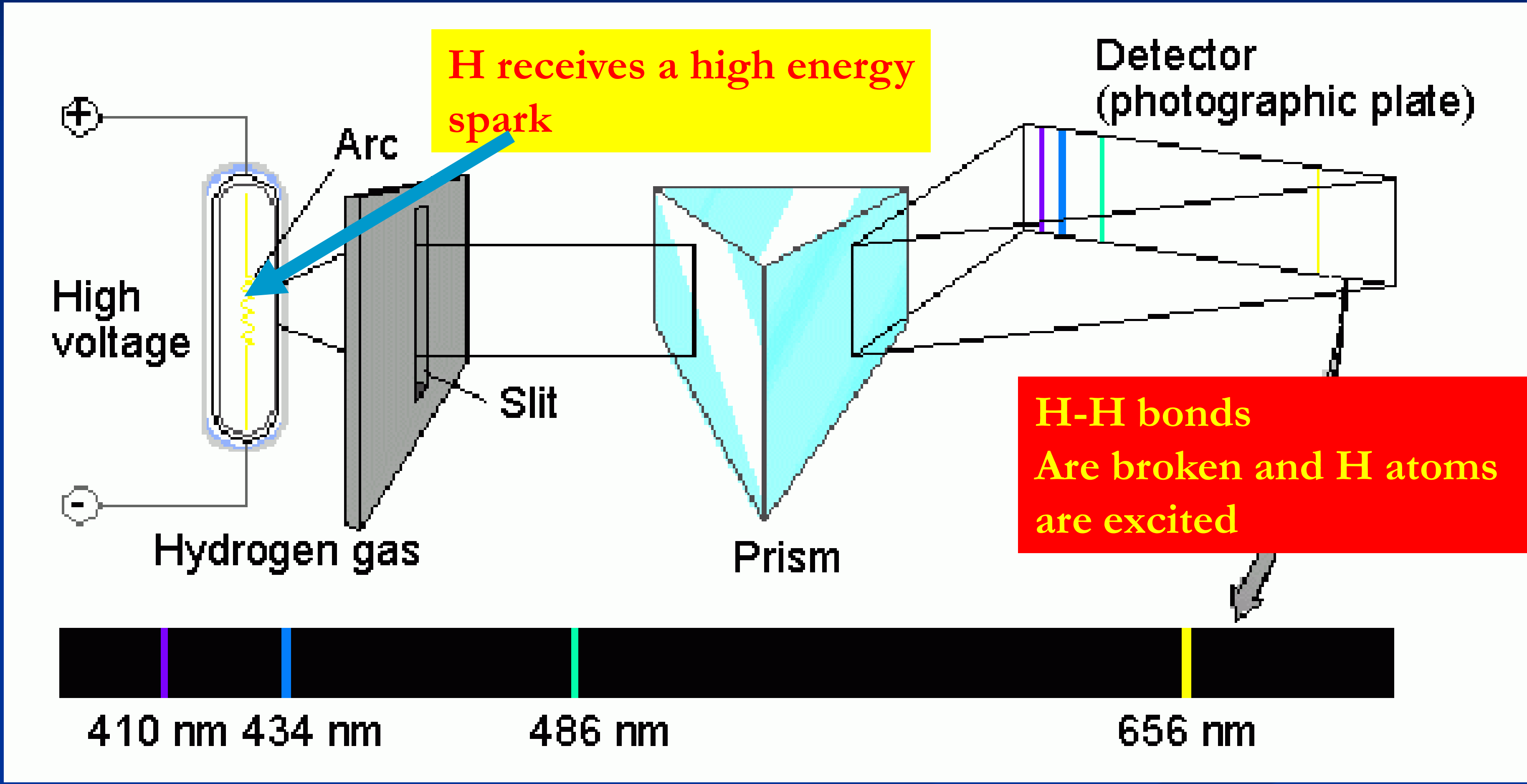
Bright-line Spectra



The Line Spectrum of Hydrogen

- Main experiments led to the information related to atom:
    - Thompson discovery of electron
    - Rutherford discovery of nucleus
    - Study of emission of light by excited hydrogen atom
- When H_2 molecules absorb energy, some H-H bonds are broken and excited H-atoms will be produced
- The excited H-atoms release energy by emitting light at various wavelengths that is known as emission spectrum of H-atoms

Spectroscopic analysis of the hydrogen spectrum…



H receives a high energy spark

H-H bonds
Are broken and H atoms are excited

Hydrogen emission spectrum is called “line spectrum”

Line Spectrum of Hydrogen

- The *Rydberg equation*

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

- **Balmer** (initially) and **Rydberg** (later) developed the equation to calculate all spectral lines in the hydrogen spectrum
- *Rydberg constant = 1.09737316 m^{-1}*
- n_1 and n_2 are positive integers where $n_2 > n_1$.

Significance of the line spectrum of H-atom

- Only certain energies are allowed for the electron in the hydrogen atom
- That is, the energy of an electron in a hydrogen atom is quantized.
- Changes in energy between discrete energy levels in hydrogen will produce only certain wavelengths of emitted light.
- The discrete line spectrum of hydrogen shows that only certain energies are possible.
- The electron energy levels are quantized. If all energy levels are allowed the spectrum would be continuous

The Bohr Model

- Niels Bohr (Danish physicist) 1885-1962
- Developed a quantum model

  for H atom that explained the emission line spectrum
- Electron moves around the nucleus only in certain allowed circular paths called orbits, in which it has a certain amount of energy
- The electrons were attracted to the nucleus because of opposite charges.
- But electron does not fall in to the nucleus because it is moving around and it does not radiate energy.

The Bohr Atom

- **Only valid energies for hydrogen's electron are allowed with the following equation**
- **The energies that the electron in a hydrogen atom can possess is given by the equation:**

$$E_n = -2.18 \times 10^{-18}\,\mathrm{J}\left(\frac{1}{n^2}\right)$$

n is an integer= 1, 2, 3, ..

- Negative sign means that the energy of electron bound to nucleus is lower than it would be if it were at infinite distance ($n = \infty$) from the nucleus.
  - The energy of an electron in an atom is lower than that of the free electron

- The quantity of energy absorbed or emitted depends on the difference of energy levels between initial and final state.
- The higher the excited state, the farther away the electron from nucleus and the less tightly is held by nucleus.
- E=0 is set at an distance of ∞ away from the nucleus and becomes more negative as the electron comes closer to the nucleus

$$E_n = -2.18\times10^{-18}\,\mathrm{J}\left(\frac{1}{\infty^2}\right) = 0$$

- An electron can pass only from one orbit to another. Absorption or emission of E will occur
- Putting Energy into the atom moves the electron away from the nucleus.
  - From ground state to excited state.
- When it returns to ground state it gives off (emits) light of a certain energy.
- Ground state is the most stable one. The stability diminishes when (n) increases
- Wavelength of a photon released or absorbed can be calculated by using the equation

$$\boxed{\Delta E = h\upsilon = h\frac{c}{\lambda}} \quad \Rightarrow \quad \boxed{\lambda = \frac{hc}{\Delta E}}$$

For a mole of hydrogen atom in the ground state

$$E_n = -2.178\, X\, 10^{-18} \frac{J}{particle}\, X\, \frac{6.02\, X\, 10^{23}\, particles}{1 mol}\, X\, \frac{1 kJ}{1000\ J}\, X\, \frac{1}{n^2} = \frac{-1312\, kJ / mol}{n^2}$$

$$E_n = \frac{-1312\, kJ}{n^2\, mole}$$

Bohr’s theory explains the line spectrum of hydrogen

- Each spectral line in the hydrogen spectrum corresponds to a specific transition from one orbit to another
- Electrons moving from ground state to higher states require energy; an electron falling from a higher to a lower state releases energy

Calculation of the emitted or absorbed radiation

- Bohr's equation can be used to calculate the energy of the transitions within the H atom

$$\Delta E = -2.18\times10^{-18}\,\mathrm{J}\left(\frac{1}{n_f^{\,2}}-\frac{1}{n_i^{\,2}}\right)$$

- **When $n_i > n_f$ a photon is emitted; the term in parenthesis is positive and ΔE is negative; the energy is released**
- **When $n_f > n_i$ a photon is absorbed; the term in parenthesis is negative; ΔE is positive; the energy is absorbed**

Calculation of the wavelength of the emitted or absorbed radiation (emission or absorption line)

$$\Delta E = -2.18\times10^{-18}\,\mathrm{J}\left(\frac{1}{\mathrm{n_f}^2}-\frac{1}{\mathrm{n}_i{}^2}\right)$$

- **Since**

$$\Delta E = h\upsilon = h\frac{c}{\lambda}$$

$$\frac{1}{\lambda} = \frac{2.18\times10^{-18}\,\mathrm{J}}{\mathrm{hc}}\left(\frac{1}{\mathrm{n_f}^2}-\frac{1}{\mathrm{n}_i{}^2}\right)$$

Since λ can only be positive, the absolute value is used

Energy Transitions

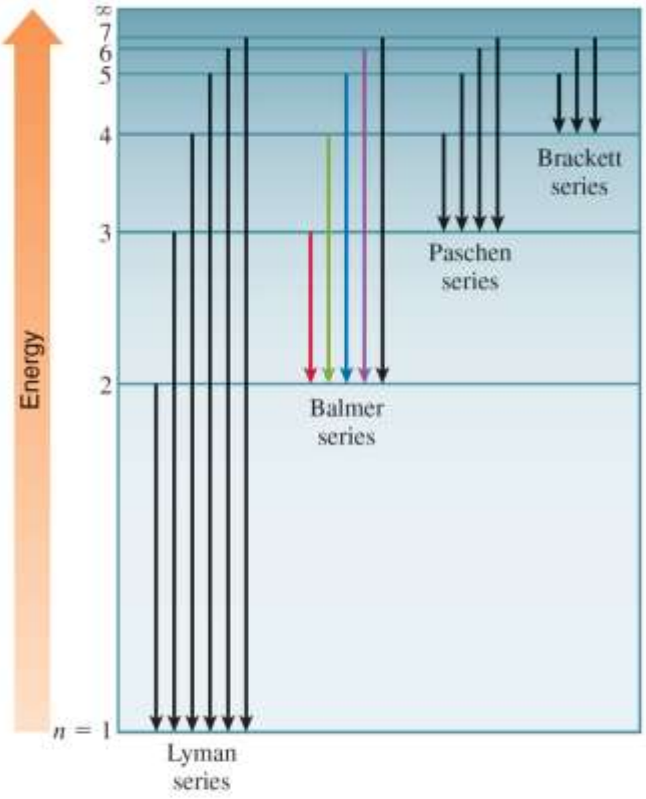
Calculate the energy needed for an electron to move from *n* = 1 to *n* = 4.

$$\Delta E = -2.18 \times 10^{-18}\,\mathrm{J}\left(\frac{1}{4^2} - \frac{1}{1^2}\right)$$

$$\Delta E = -2.04\times 10^{-18}\,\mathrm{J}$$

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



Example 1

Calculate the energy required to move the hydrogen electron from n=1 to n=2. Find the wavelength of radiation that had to be absorbed by the electron.

$$\Delta E = -2.178\times10^{-18} J\left(\frac{1}{n_f^{\,2}} - \frac{1}{n_i^{\,2}}\right)$$

$$\Delta E = -2.178\times10^{-18} J\left(\frac{1}{2^2} - \frac{1}{1^2}\right) = 1.633\times10^{-18} J$$

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.626\times10^{-34} J\cdot s)(2.9979\frac{m}{s})}{1.633\times10^{-18} J}$$

$$\lambda = 1.216\times10^{-7} m \times \frac{10^9 nm}{1m} = \boxed{121.6nm}$$

Example 2

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

$$\Delta E = -2.178\times10^{-18}\,J\left(\frac{1}{n_f^{\;2}} - \frac{1}{n_i^{\;2}}\right)$$

$$\Delta E = -2.178\times10^{-18}\,J\left(\frac{1}{\infty} - \frac{1}{1^2}\right)$$

$$\Delta E = -2.178\times10^{-18}\,J(0-1) = \boxed{2.178\times10^{-18}\,J}$$

Energy was absorbed by the electron so the **value of ΔE value is positive.**

6.4 Wave Properties of Matter

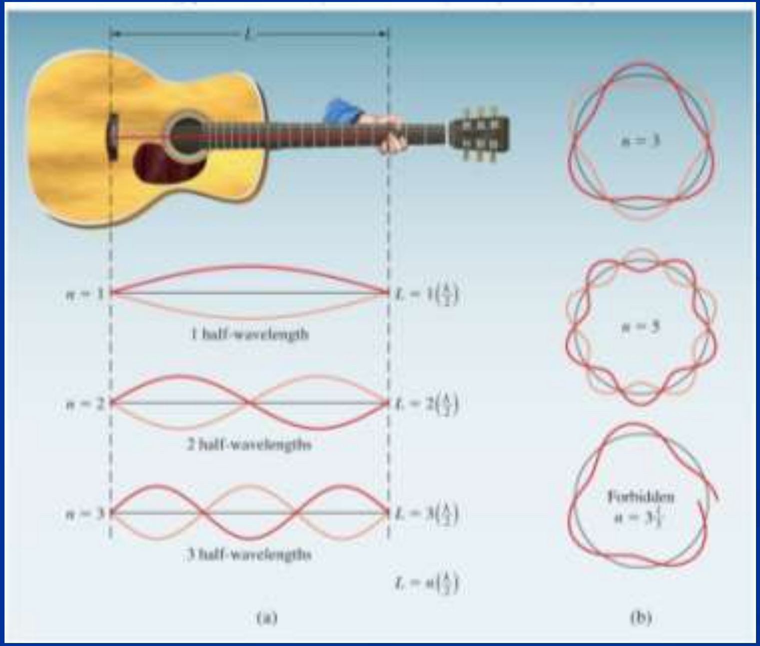
- Bohr could not explain why electrons were restricted to fixed distances around the nucleus
- Louis de Broglie (1924) reasoned that if energy (light) can behave as a a stream of particles (photons) then perhaps particles (electrons) could exhibit under certain circumstances wavelike properties

The electron propagates through space as an energy wave. To understand the atom, one must understand the behavior of electromagnetic waves.

Louis deBroglie

Wave Properties of Matter

- De Broglie proposed that electrons in atoms behave as standing waves
- There are some points called nodes (where the wave exhibits no motion at all)



Wave Properties of Matter

- De Broglie's idea of particle and wave properties are related by the following

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

where λ = wavelength

m = mass (kg)

u = velocity (m/s)

Calculate the de Broglie wavelength of the "particle" in the following

A 25.0 g bullet traveling at 612 m/s. Note: 1 Joule = 1 kg · m^2/s^2

Planck's constant, h = 6.63X10^{-34} J.s = 6.63X10^{-34} kg · m^2/s

$$\lambda = \frac{h}{mu} = \frac{6.63X10^{-34}\,kg.m^2/s}{(0.025kg)(612m/s)} = 4.3X10^{-35}m$$

$$\lambda = \frac{h}{mu} = \frac{6.63X10^{-34}\,kg.m^2/s}{(9.109X10^{-31}\,kg)(63m/s)} = 1.16X10^{-5}m$$

Shortcomings of Bohr Model

- problems:
  - did not work for other atoms of more than one electron
  - did not explain chemical behavior of atoms
  - Electron appears to behave as a particle in some circumstances and as a wave in otheres. No description could explain the behavior of electrons in atoms

6.5 Quantum Mechanics

- Scientists were eager to understand exactly where electrons are in an atom.
- **Heisenberg's uncertainty principle** mathematically described the position and velocity of an electron. The more you know about one, the less you are sure about the other quantity.

Heisenberg’s Uncertainty Principle

- According to de Broglie: Electron behaves like a wave
- Is it possible to specify the position of a wave at a particular instant?
- Energy, wavelength and amplitude can be determined
- <u>But exact position is impossible to be determined</u>
- The electron cannot be imagined as :
  - moving particle
  - In a path of the same radius (well defined orbits)
- Thus, location, direction and speed of motion of a particle cannot be determined
- Then Bohr Model had to be “Abandoned

Heissenberg Uncertainty Principle

"It is impossible to determine both the position and momentum of a subatomic particle (such as the electron) with arbitrarily high accuracy"

- The effect of this principle is to convert the laws of physics into statements about relative, instead of absolute, certainties.

Heisenberg Uncertainty Principle

- we cannot know the exact position and momentum (motion) of the electron
- as more is known about position, less is known about momentum
- uncertainties are inversely proportional

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

where

Δx: uncertainty in measuring position

$\Delta\upsilon$: uncertainty in measuring velocity

- ➢ minimum uncertainty is h/4π

Quantum Mechanics

- Heisenberg's equation disproved Bohr's model of defined orbits for electrons
- Bohr's theory did not provide a clear description
- Erwin Schrödinger, derived a complex mathematical formula to incorporate wave and particle characteristics

Quantum Mechanics

- Exact position of electron can not be defined
  - Exact bath of electron about nucleus can not be defined
- Werner Heisenberg, Louis de Broglie and Erwin Schrodinger made the approach called "Quantum Mechanics"
- They assumed that the electron is a standing wave

The Quantum Mechanical Model

- Waves are associated with electrons
- Information about energies of electrons and their positions are obtained from studying the associated waves
- Description of electron is based upon

  " Probability of finding a particle within a given region of space" " but not on the exact position"

Schrödinger Equation

- Wave equation describing electron as being a wave
- The amplitudes (height), Ψ, of electron wave at various points of space are calculated
- Ψ commonly called "wave function"
- Ψ provides information about the allowable energies for an electron in H atom.
- Ψ corresponds to a certain energy and describes a region around nucleus "Orbital" where the electron having that energy may be found

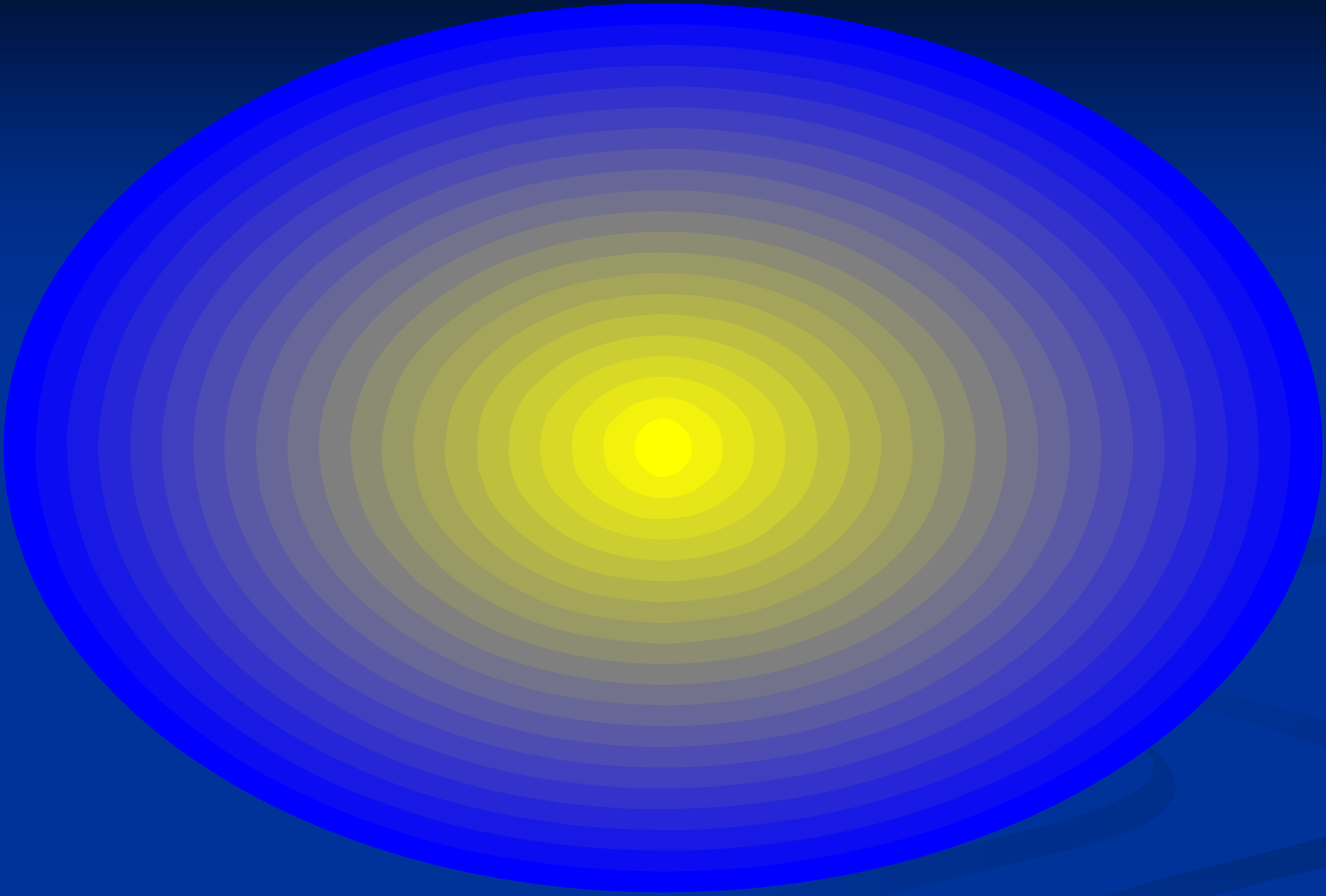
- **Orbital:** Region around the nucleus where the electron can be expected to be found
- The Function Ψ^2 (Ψ = psi)

  Ψ^2 describes the probability of the position of the electron at a particular point
- Ψ^2 α Probability of finding a particle in a given region of space
- Ψ^2 α Electric charge density at a given region of space

Thus,

- The charge can be assumed to be spread out as a charge cloud by rapid motion of electron
- The cloud is denser in some regions than others

- The probability of finding electron in a given region in space is proportional to the density of the cloud



Quantum Mechanics

- Quantum mechanics (wave mechanics) does not allow us to specify exact location of electrons, we can predict high probability of finding an electron
- Use the term atomic orbital instead of "orbit" to describe the electron's position within the atom

6.6 Quantum Numbers

- There are many solutions to Schroedinger’s equation for H atom
- Each solution is a wave function called **Orbital**.
- Each orbital can be described with **quantum numbers** that describe the distribution of electron density in an atom

- The first three quantum numbers come from the Schrödinger equation :
  - **Principal quantum number main**
  - **Angular momentum quantum number**
  - **Magnetic quantum number**
- **The 4th quantum number is the electron spin quantum number**

Principal quantum number (n)

- It designates the size of the orbital
- Integer values: 1,2,3, and so forth
- The value of (n) determines the energy of an orbital
- The larger the "*n*" value, the greater the average distance from the nucleus
- Correspond to quantum numbers in Bohr's model

Angular momentum quantum number (l)

- It describes the shape of the atomic orbital
- Integer values: 0 to $n - 1$
- The number of possible shapes (or l values) for an energy level is equal to ***n***
- The possible values of l are 0 and all positive integers less than or equal to $n - 1$

- **l has integer values from 0 to n-1**
  - l = 0 is called s
  - l = 1 is called p
  - l =2 is called d
  - l =3 is called f
  - l =4 is called g
- A collection of orbitals with the same value of n is frequently called a shell.
- One or more orbitals with the same n and l are referred to as subshell.
- The shell of n =2 is composed of two subshells l=0 and l =1

Magnetic Quantum Number, m_l

- m_l indicates the orientation of the orbital in space relative to the other orbitals in the atom
- m_l has integer values from $+l \rightarrow -l$ *including 0*
- The number of m_l values indicates the number of orbitals in a subshell with a particular l value (ech m_l refers to a different orbital)
- each orbital holds maximum of **2 electrons**
- total number of orbitals in a shell is equal to n^2

Allowed values of quantum numbers

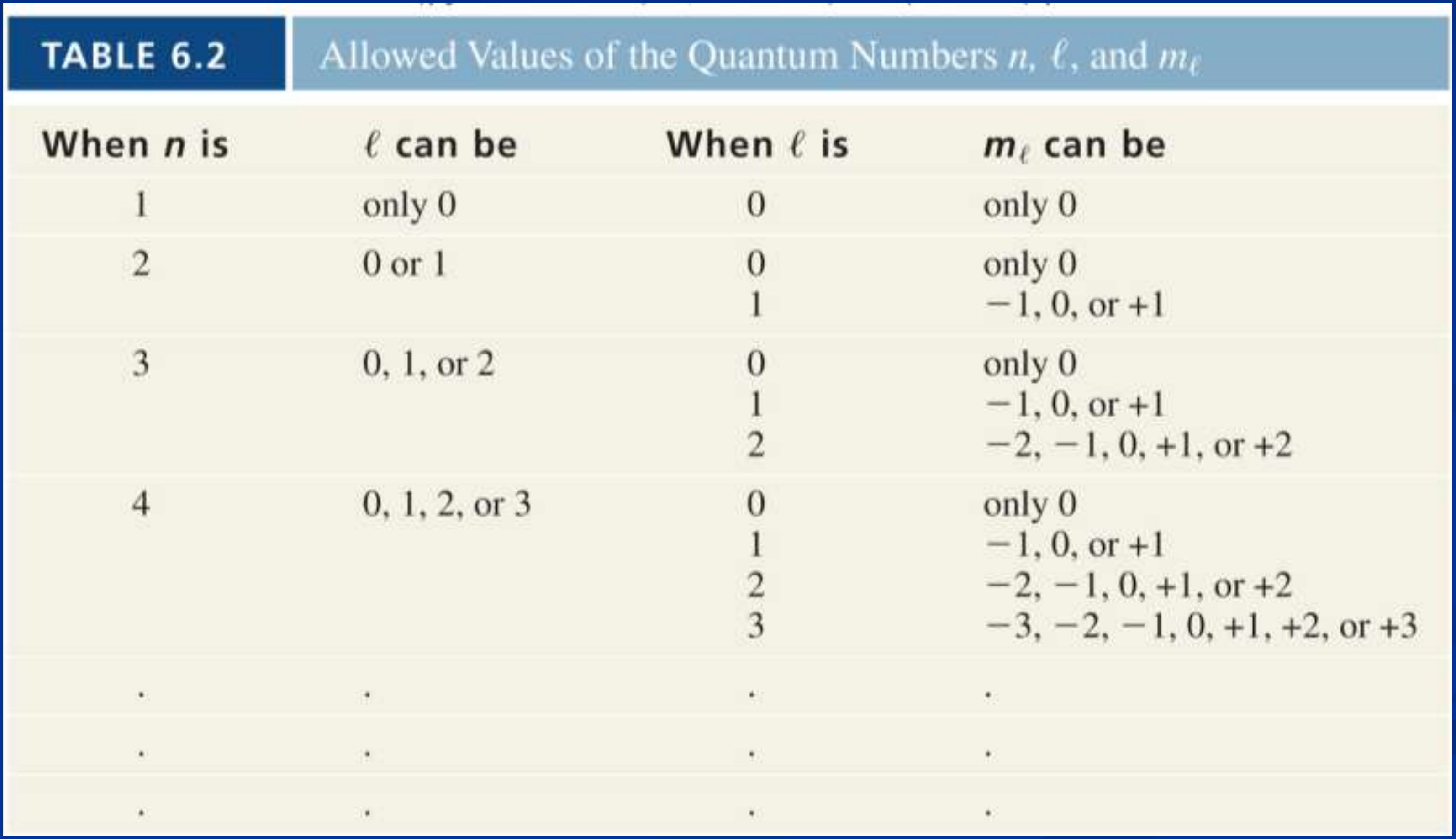


TABLE 6.2 Allowed Values of the Quantum Numbers n, ℓ, and m_ℓ

When n is	ℓ can be	When ℓ is	m_ℓ can be
1	only 0	0	only 0
2	0 or 1	0	only 0
		1	−1, 0, or +1
3	0, 1, or 2	0	only 0
		1	−1, 0, or +1
		2	−2, −1, 0, +1, or +2
4	0, 1, 2, or 3	0	only 0
		1	−1, 0, or +1
		2	−2, −1, 0, +1, or +2
		3	−3, −2, −1, 0, +1, +2, or +3
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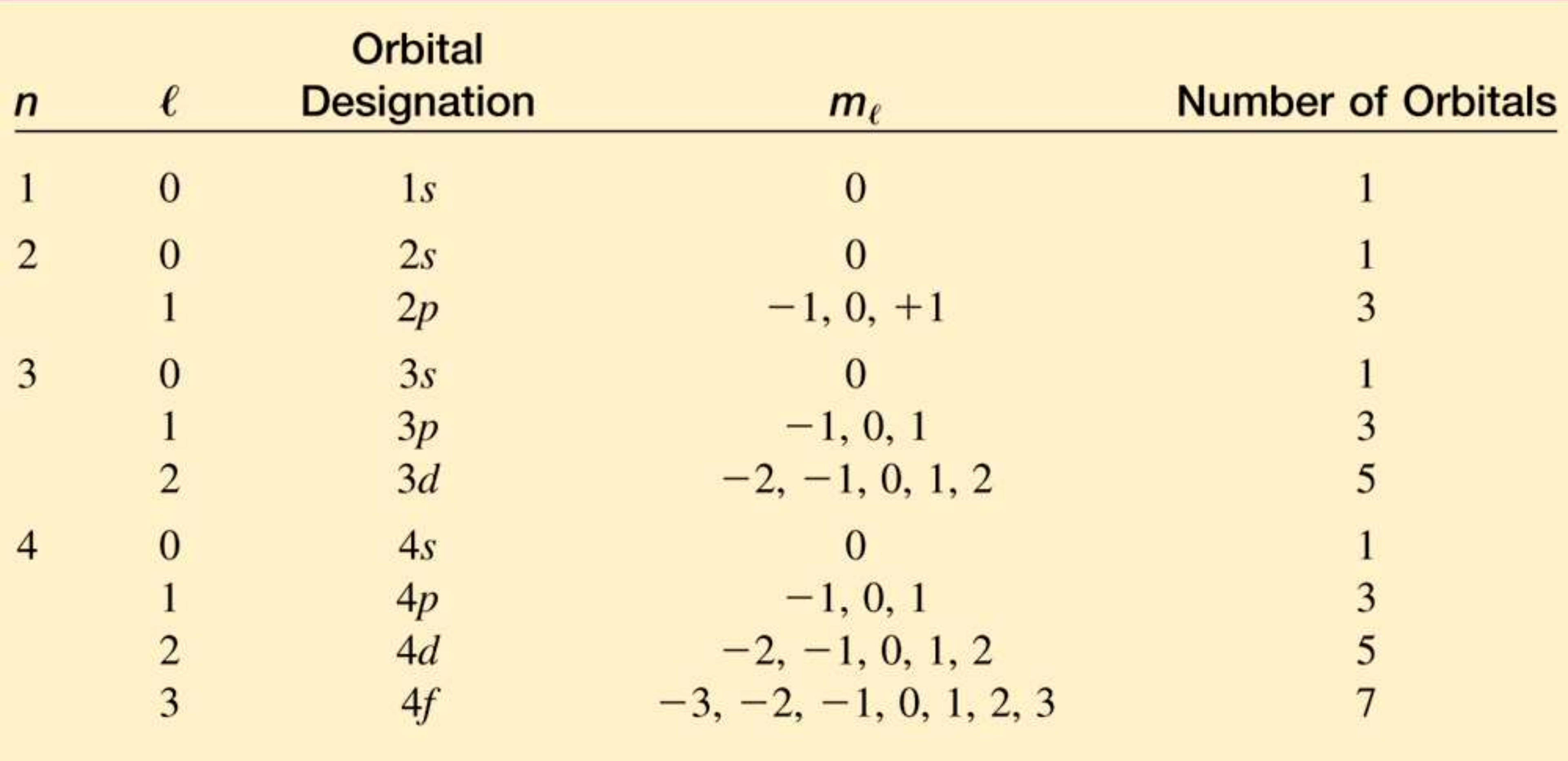
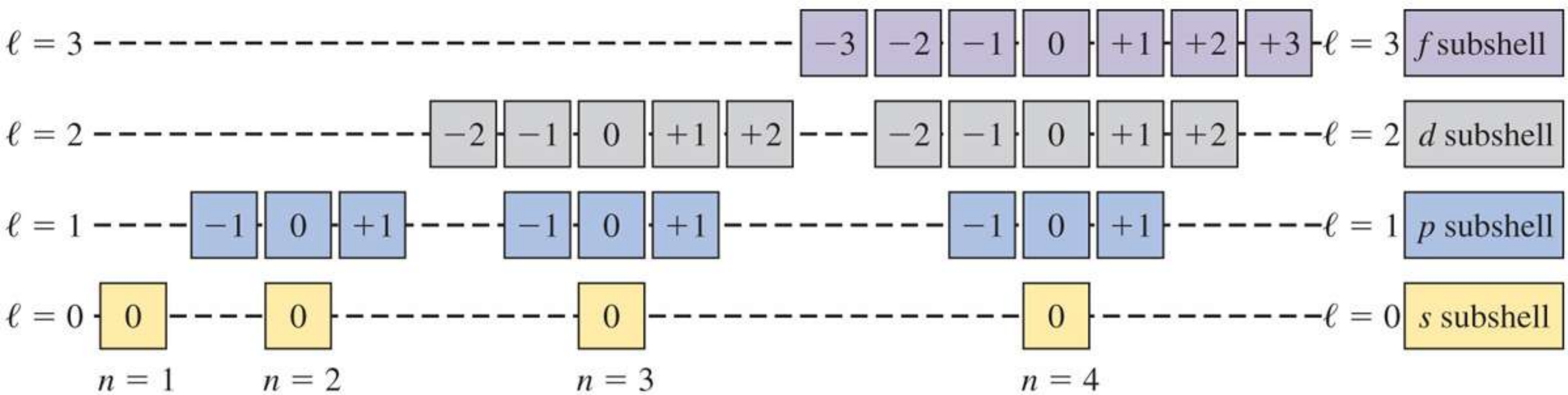
Quantum Numbers for the first four levels of orbitals in the hydrogen atom



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

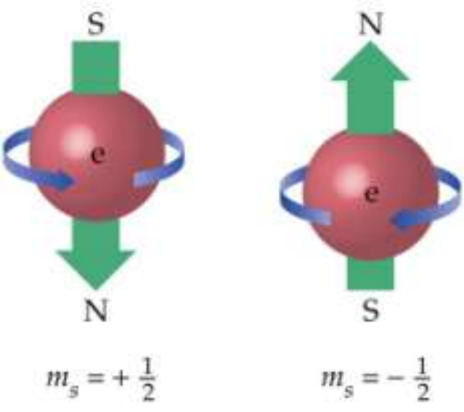
Illustration of how quantum numbers deignate shells, subshells and orbitals



Spin Quantum Number (m_s)

- When an a hydrogen atom is placed in a magnetic field each line in the emission spectrum could be split into two lines
- This was explained on the basis that the electron behaves like a tiny magnet
- m_s describes the spin of an electron that occupies a particular orbital
- The electron could have two spin states
- only 2 possible directions
- m_s can have two possible values: +½ and -½
- paired electrons must

  have opposite spins



Quantum Numbers

Which of the following are possible sets of quantum numbers?

a) 1, 1, 0, +1/2 l value not possible

b) 2, 0, 0, +1/2 possible

c) 3, 2, –2, –1/2 possible

6.7 Atomic Orbitals

(Orbital shapes and Energies)

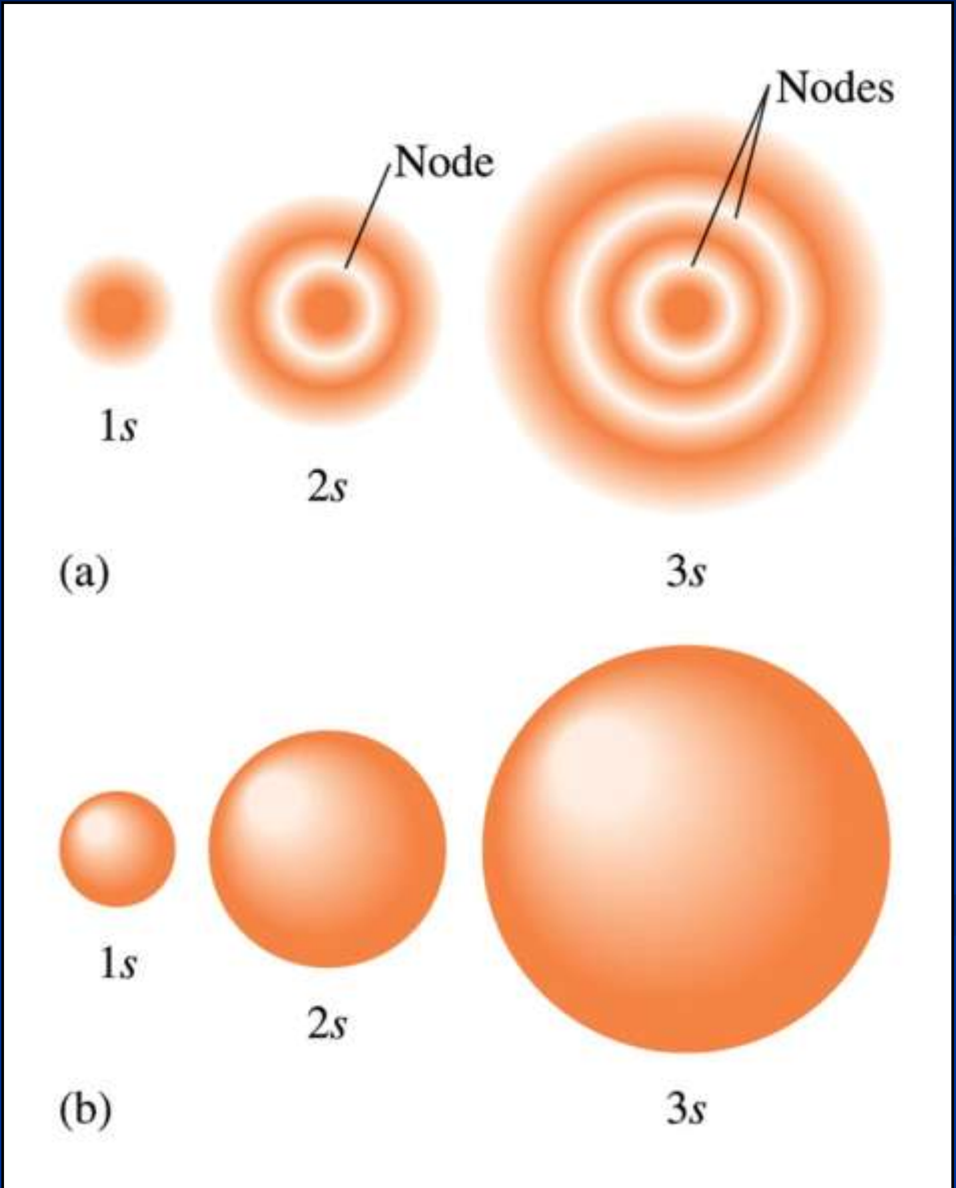
- "Shapes" of atomic orbitals
- "*s*" orbital - spherical in shape
- "*p*" orbitals - two lobes on opposite sides of the nucleus
- "*d*" orbitals - more variations of lobes
- "*f*" orbitals - complex shapes

Representations of the Hydrogen 1s, 2s, and 3s Orbitals

A. The Electron Probability Distribution

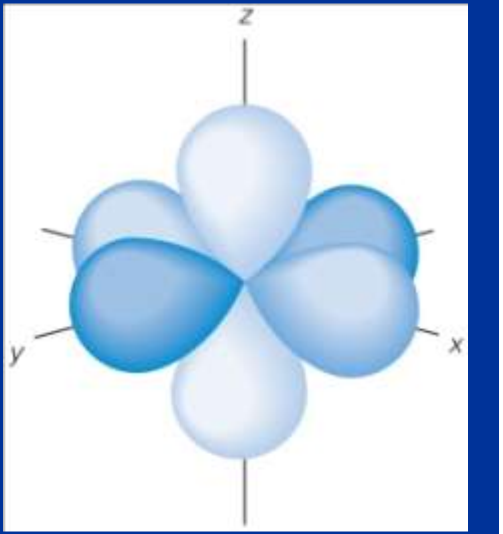
B. The surface contains 90% of the total electron probability

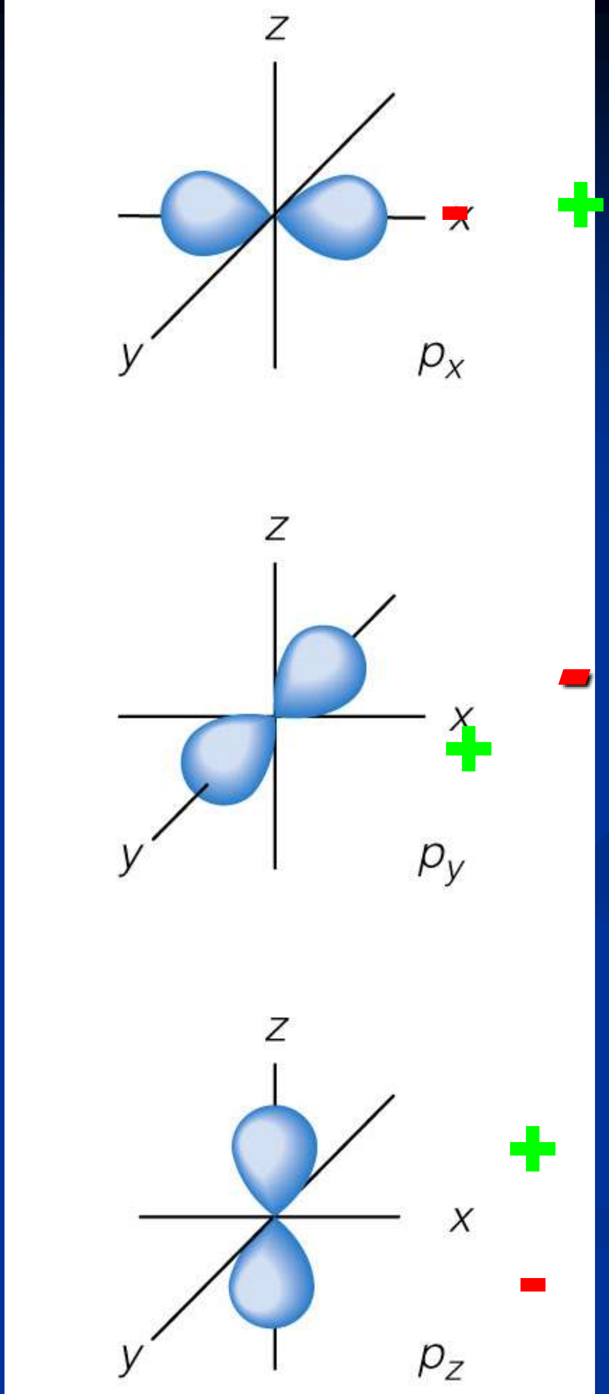
s orbitals:
1: s
spherical
***l* value of 0**



p-orbitals

Each of the Of the p orbitals is composed of 2 lobes on opposite sides of the nucleus



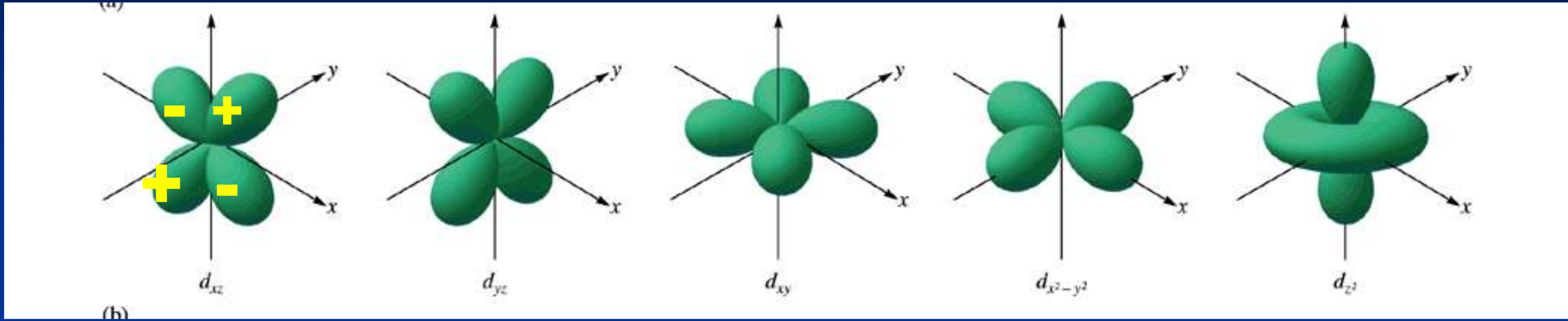


p orbitals:

- Starts from n=2
- l = 1
- $m_l = -1, 0, 1$
- Each p subshell contains 3 p orbitals

  $\underline{2p_x}$, $\underline{2p_y}$, $\underline{2p_z}$
- The three p-orbitals are identical in size, shape, and energy
- They differ only in orientation
- for n>2, shape is same but size increases

d- orbitals



d orbitals: 5: $3d_{xz}$, $3d_{yz}$, $3d_{xy}$, $3d_{x2-y2}$, d_{z2}

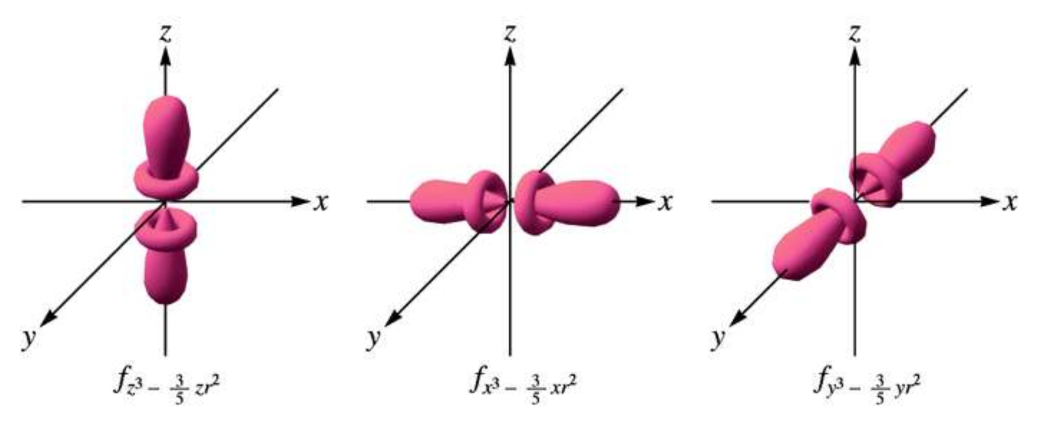
- *l* value of 2 (m_l = -2, -1, 0, 1, 2)
- 1st occur at n=3; no d-orbitals for n=1 or n=2
- for n>3, same shape but larger size

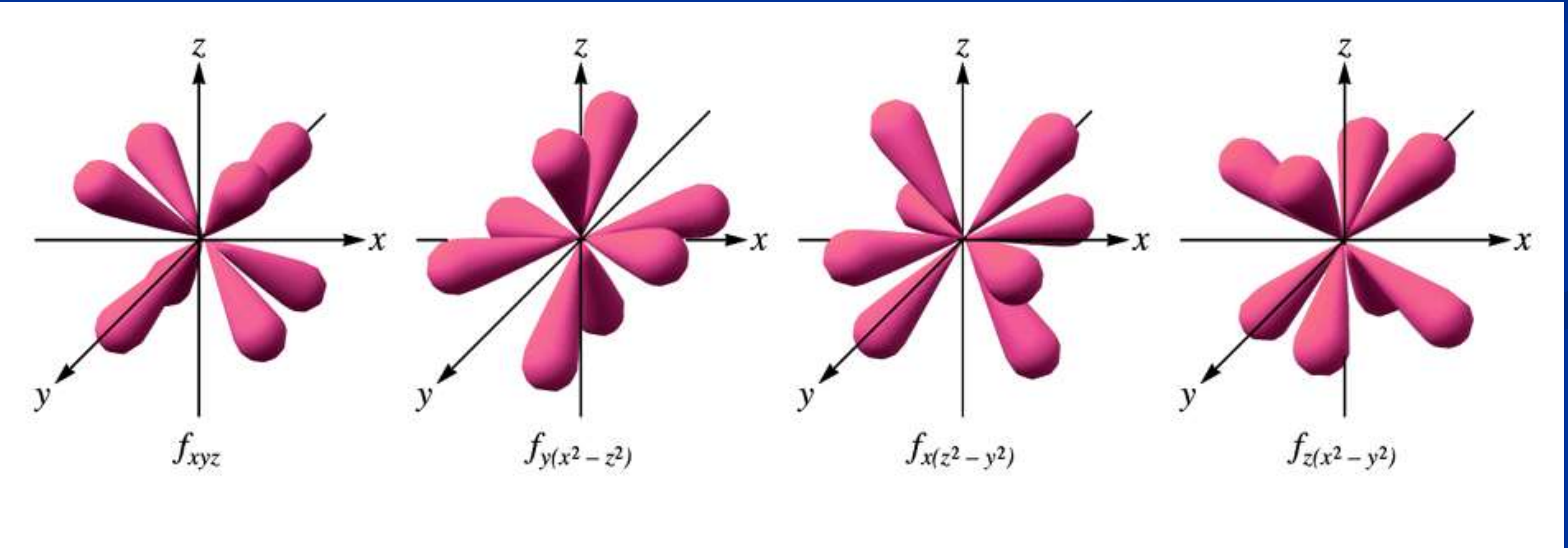
f-orbitals

f orbitals: 7 orbitals

various shapes

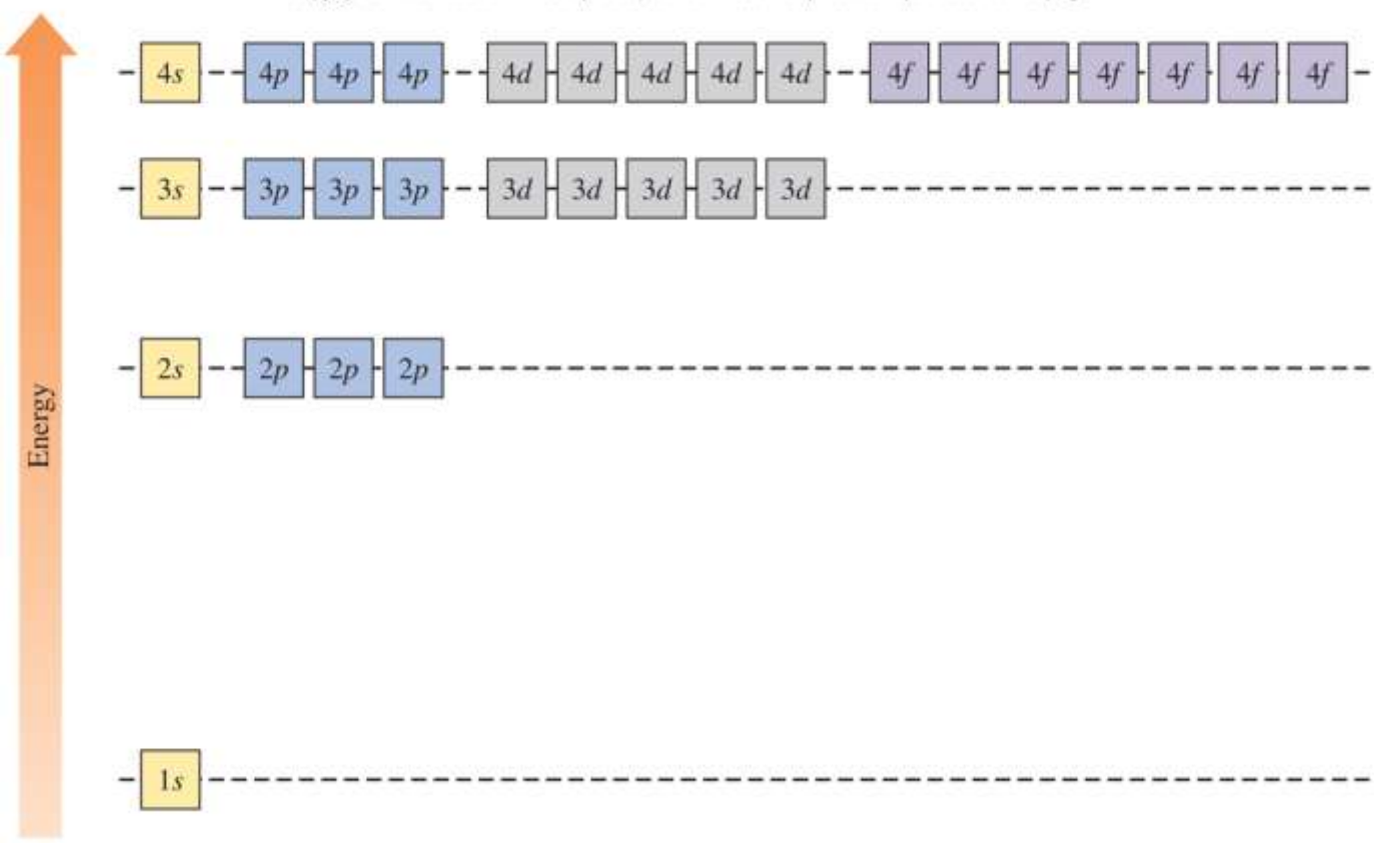
- *l* value of 3
- begin in n=4





Energies of orbitals in a hydrogen atom

- All orbitals of the same shell (n) have the same energy (they are called "degenerate") regardless of the subshell
- Energy of orbitals increases as n increases
- 1s<2s=2p<3s=3p=3d<4s=4p=4d=4f

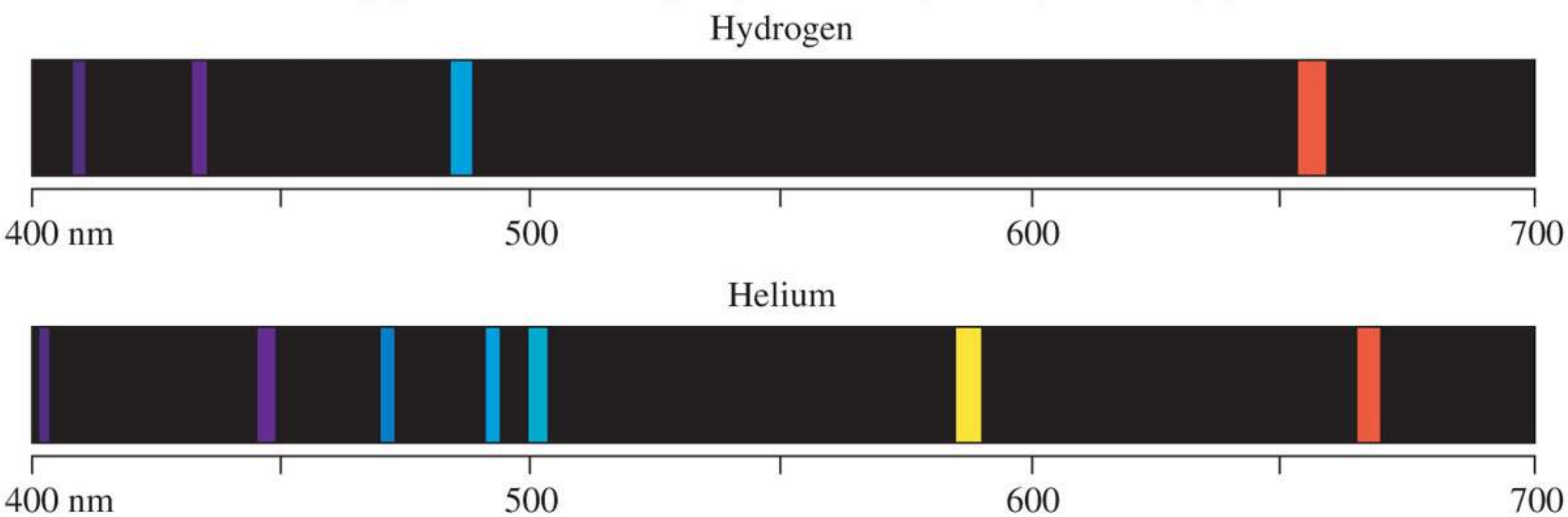


6.8 Electron Configuration

- ***Ground state*** **- electrons in lowest energy state**
- ***Excited state*** **- electrons in a higher energy orbital**
- ***Electron configuration*** **- how electrons are distributed in the various atomic orbitals**

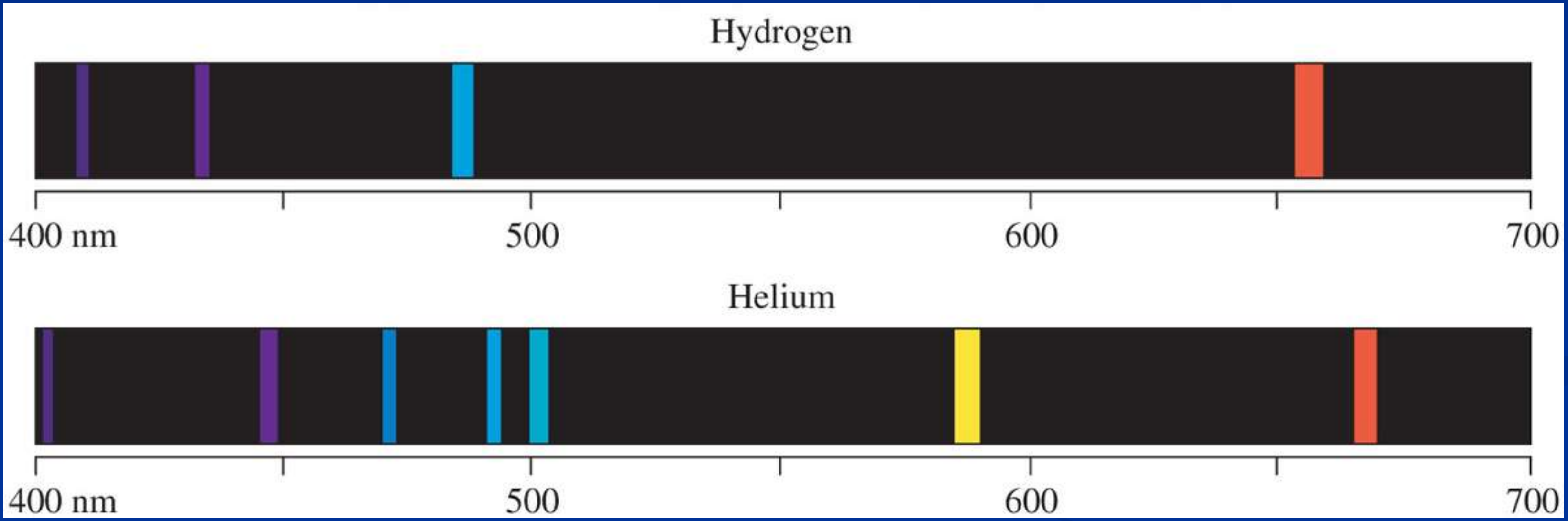
Energies of atomic orbitals in many-electron systems

- He spectrum consists more lines than the H spectrum
- Due to splitting of energy levels cuased by electrostatic interactions between heliums two electrons

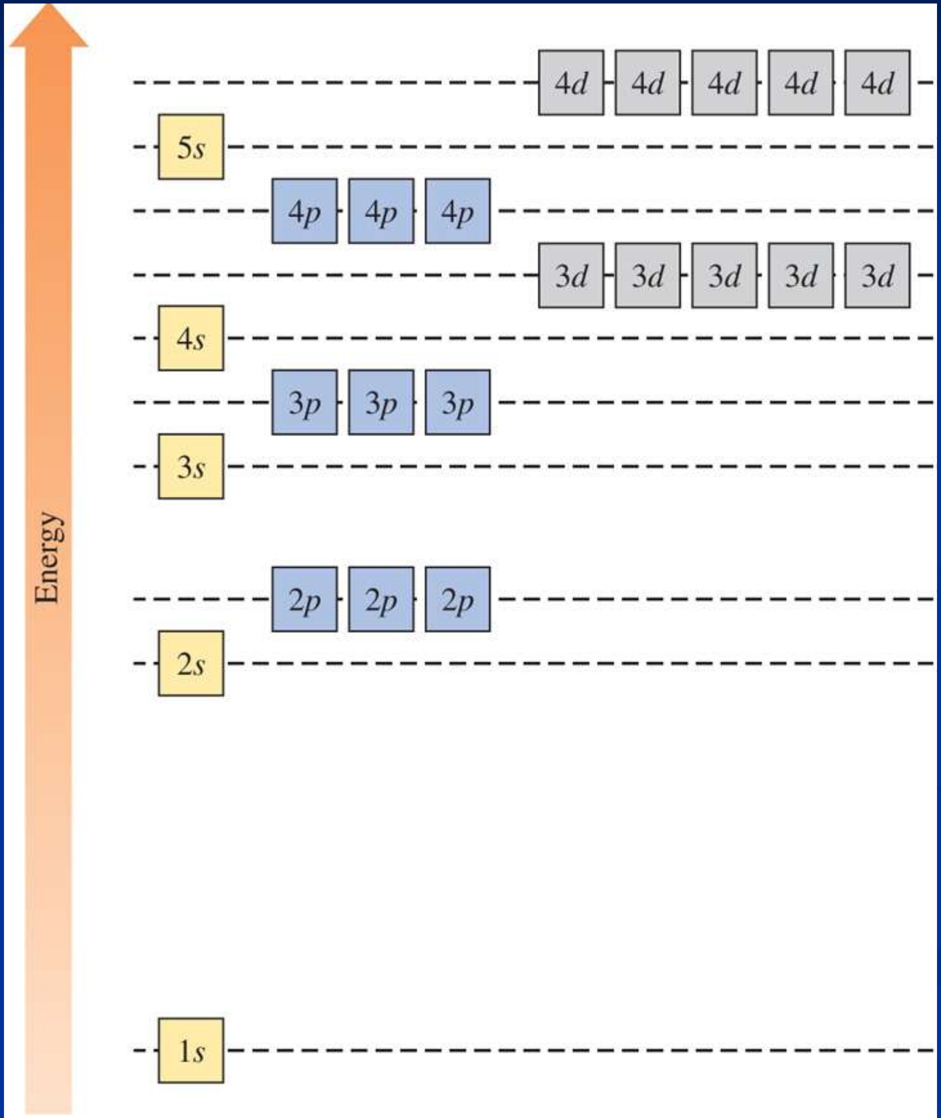


- The energy of an orbital in many-electron system depends on both the value of (n) and the value of (l).
- For a given value of (n) the energy of an orbital increases with increasing the value of (l)

Compare the Following Emission Spectra



Orbital energy levels in many-electron



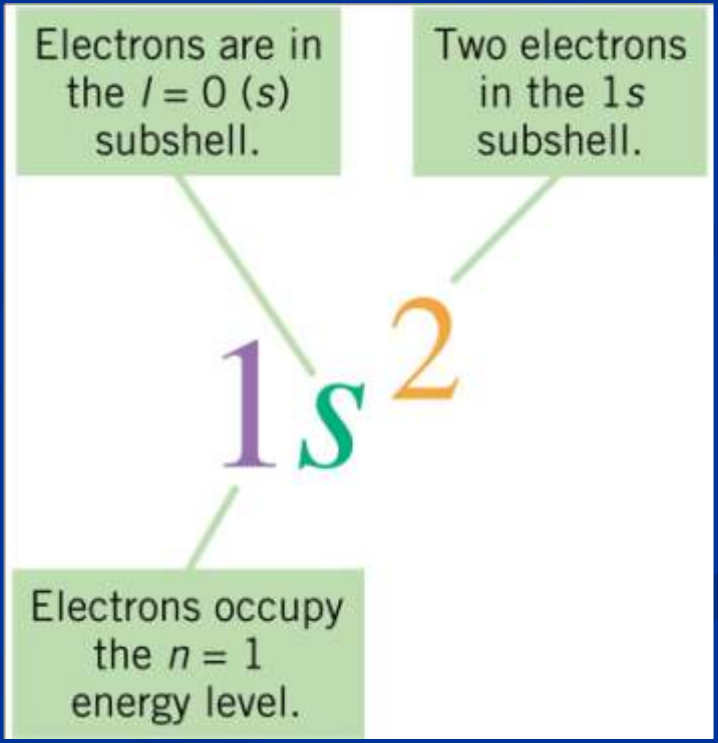
Pauli Exclusion Principle

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

Electron Configurations

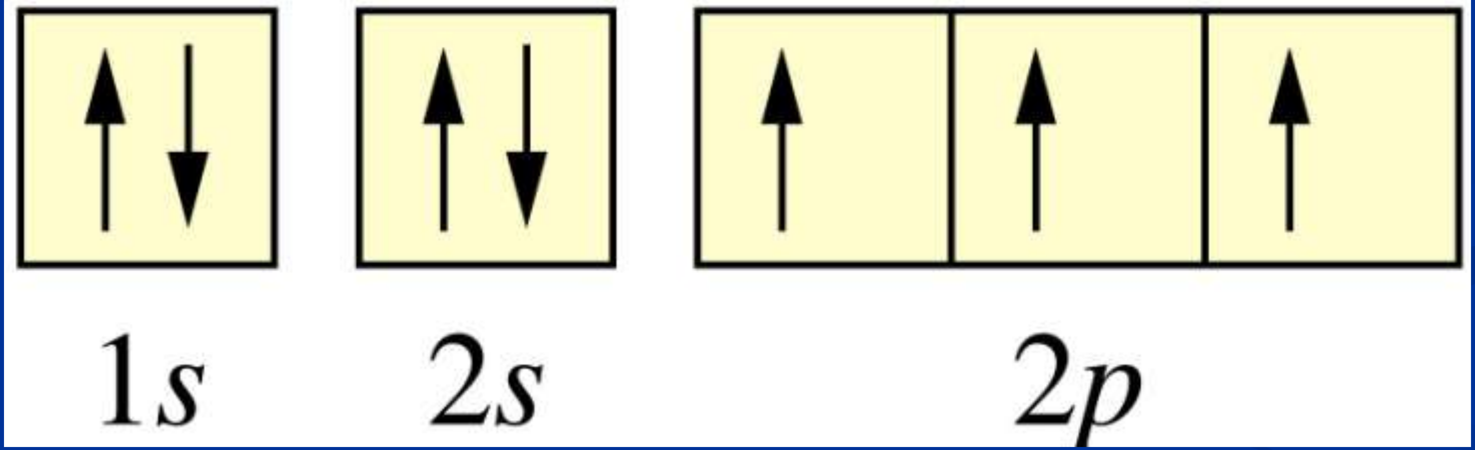
- **Electron configuration describes the distribution of electrons among the various orbitals in the atom while in the ground state**

The *spdf* notation uses numbers to designate a principal shell and the letters to identify a subshell; a superscript number indicates the number of electrons in a designated subshell



Orbital Diagrams

An orbital diagram uses boxes to represent orbitals within subshells and arrows to represent electrons:



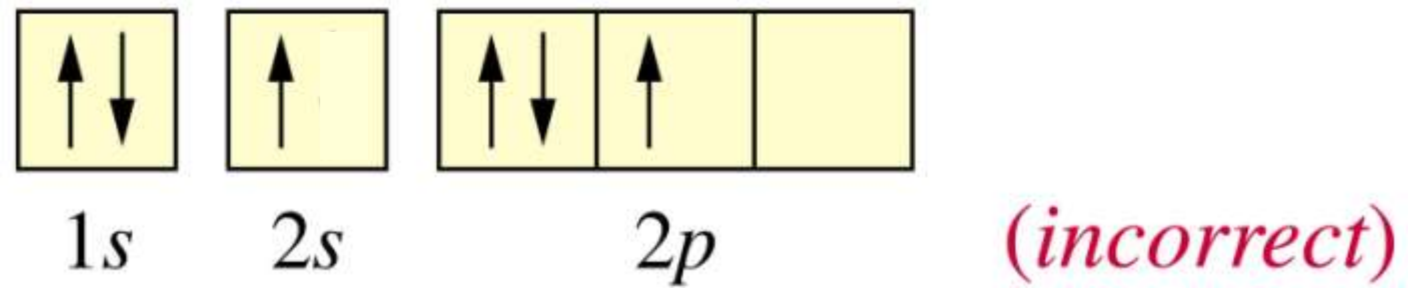
Each box has arrows representing electron spins; opposing spins are paired together

The aufbau Principle

- The way electrons are arranged in various orbitals around the nuclei of atoms.
- Aufbau is a German word means **"Building up"**
- Aufbau principle - electrons enter the lowest energy first.
  - Orbitals of different energies overlap
  -

Rules for Electron Configurations

Electrons occupy the *lowest available* energy orbitals

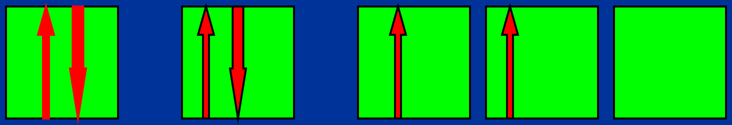


Pauli exclusion principle – <u>no two electrons in the same atom may have the same four quantum numbers</u>

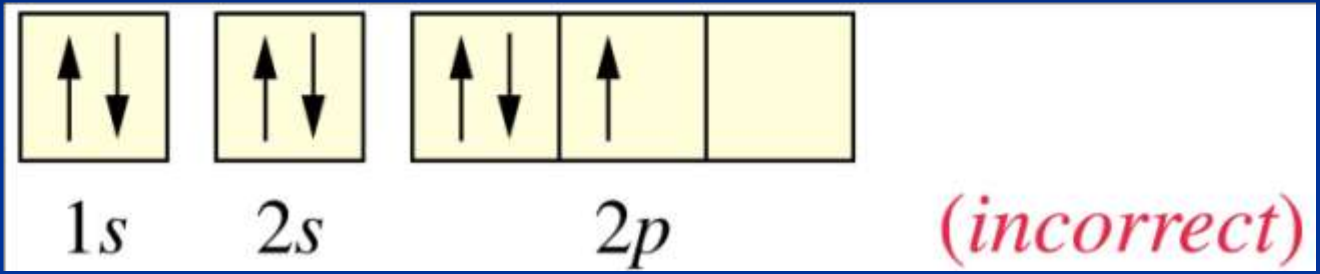
- **Orbitals hold a maximum of two electrons with opposed spins**

Hund's Rule

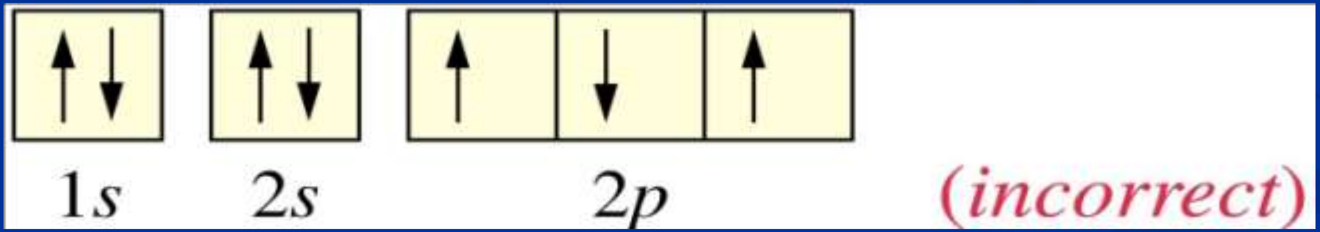
- **The most stable arrangement for electrons in orbitals of equal energy (degenerate) is where the number of electrons with the same spin is maximized**
- **For orbitals of identical energy, electrons enter empty orbitals whenever possible**
- **When electrons occupy orbitals of equal energy, they don't pair up until they have to.**
- **Example: Carbon - 6 electrons**
- $1s^2 2s^2 2p^2$



Hund’s Rule



Electrons in half-filled orbitals have parallel spins



EOS

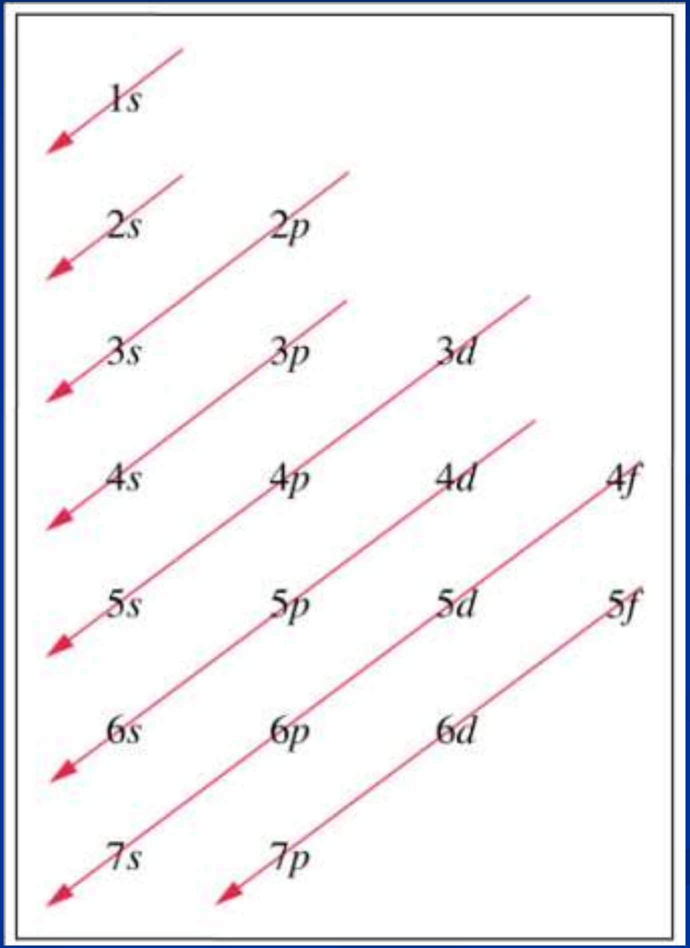
Rules for Writing Electron Configurations

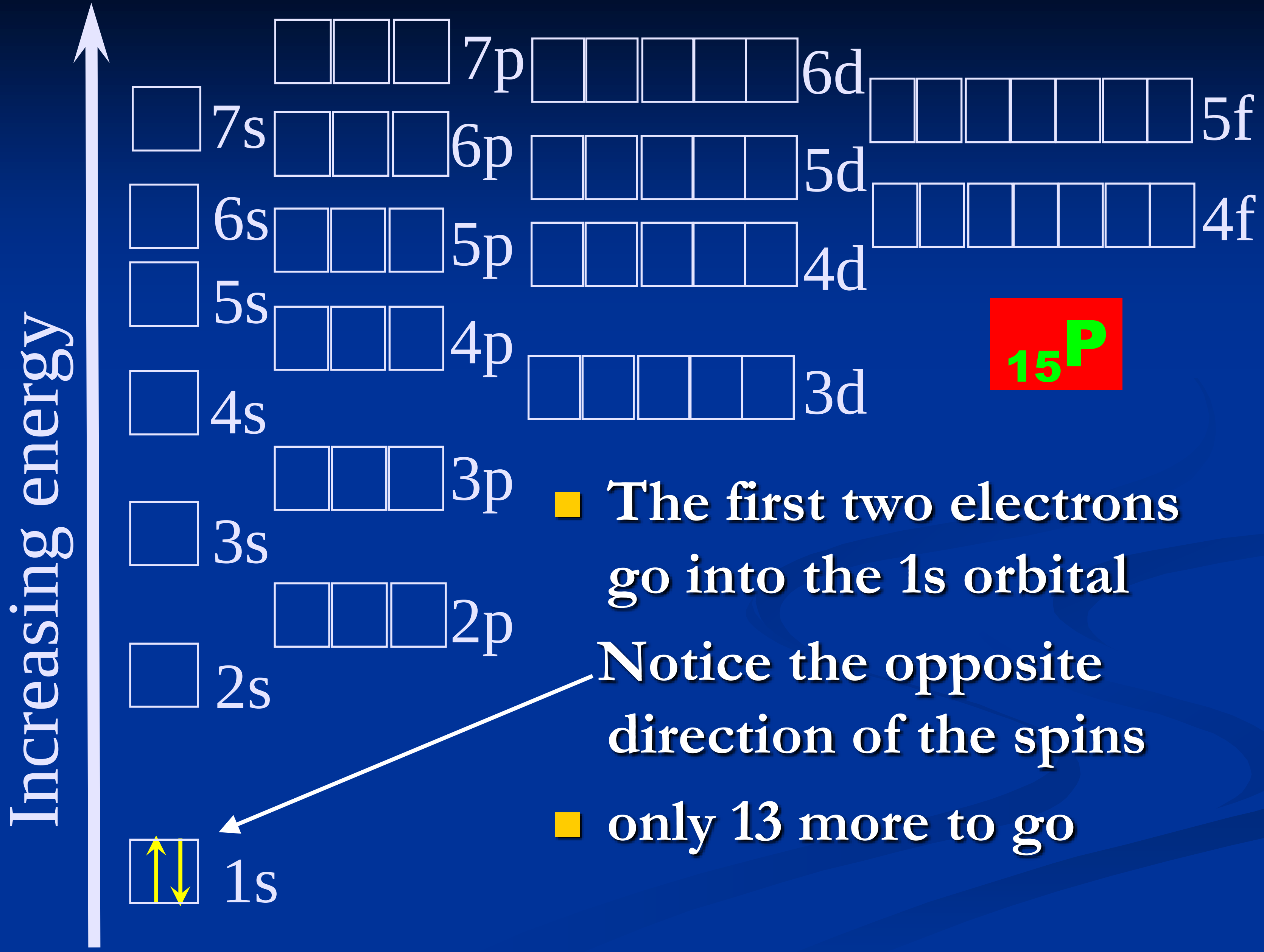
- Electrons reside in orbitals of lowest possible energy
- Maximum of 2 electrons per orbital
- Electrons do not pair in degenerate orbitals if an empty orbital is available
- Orbitals fill in order of earlier

Diagonal Rule for Electron Configurations

Subshell filling order :

Each subshell must be filled before moving to the next level



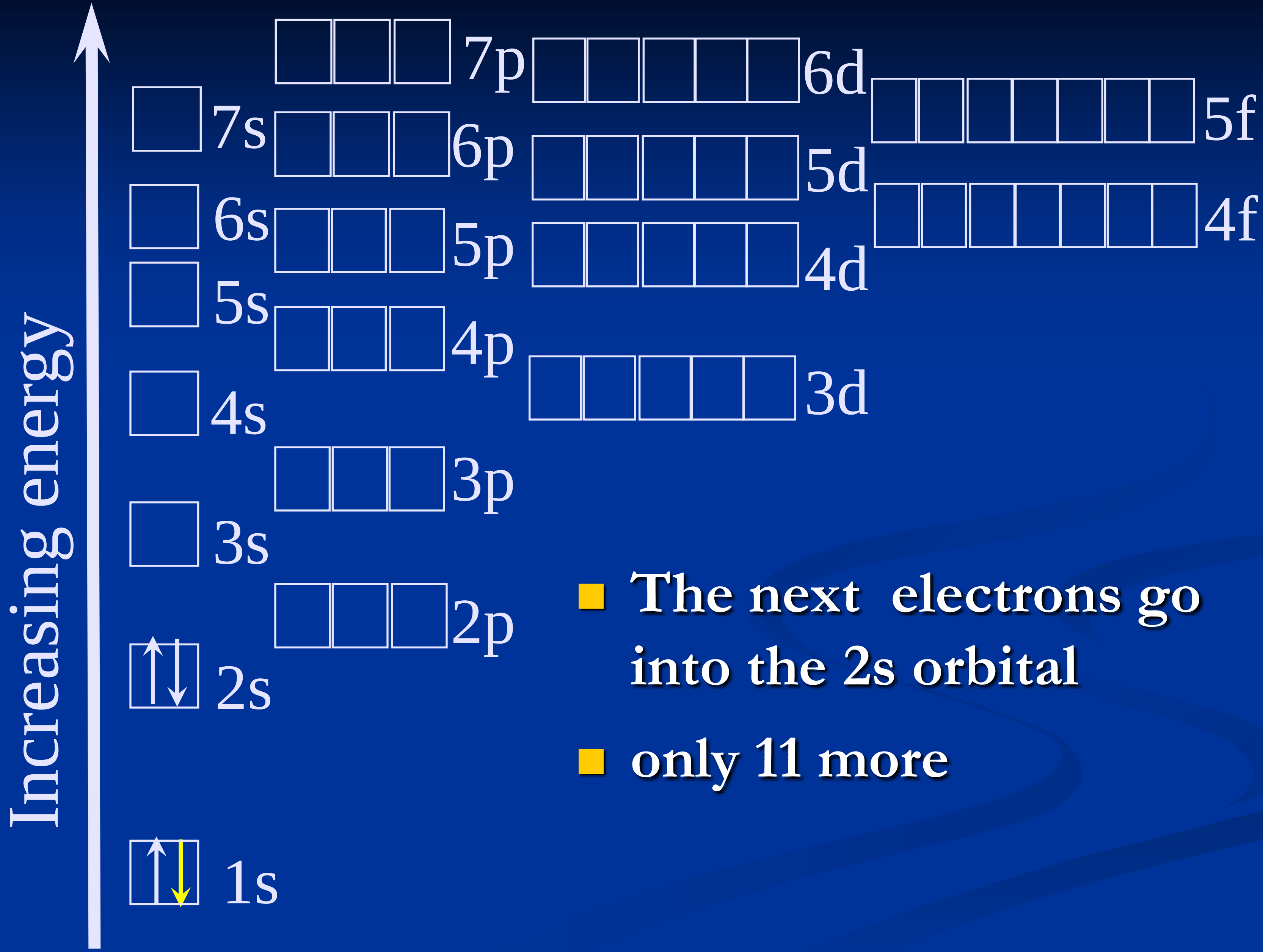


$_{15}\text{P}$

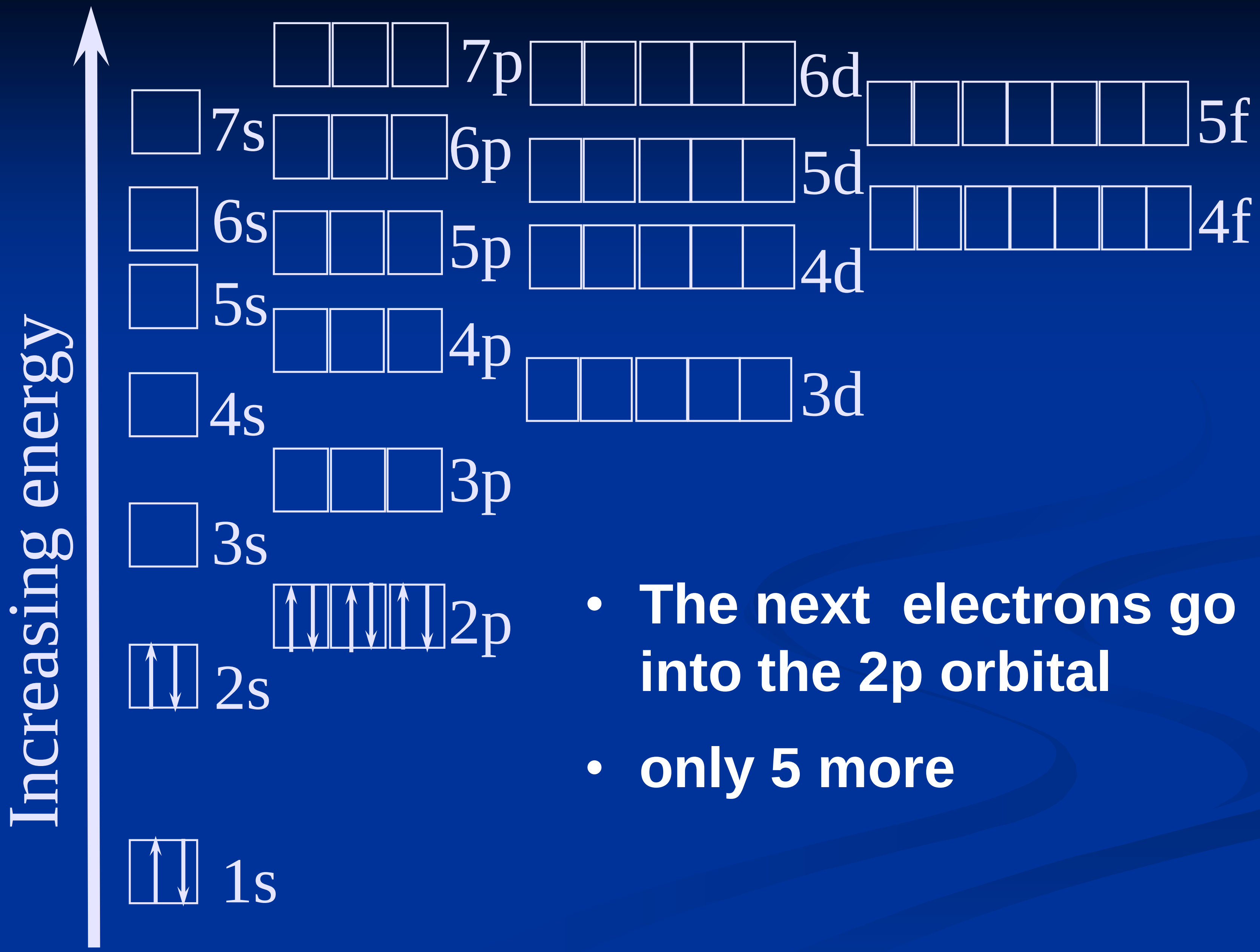
- The first two electrons go into the 1s orbital

Notice the opposite direction of the spins

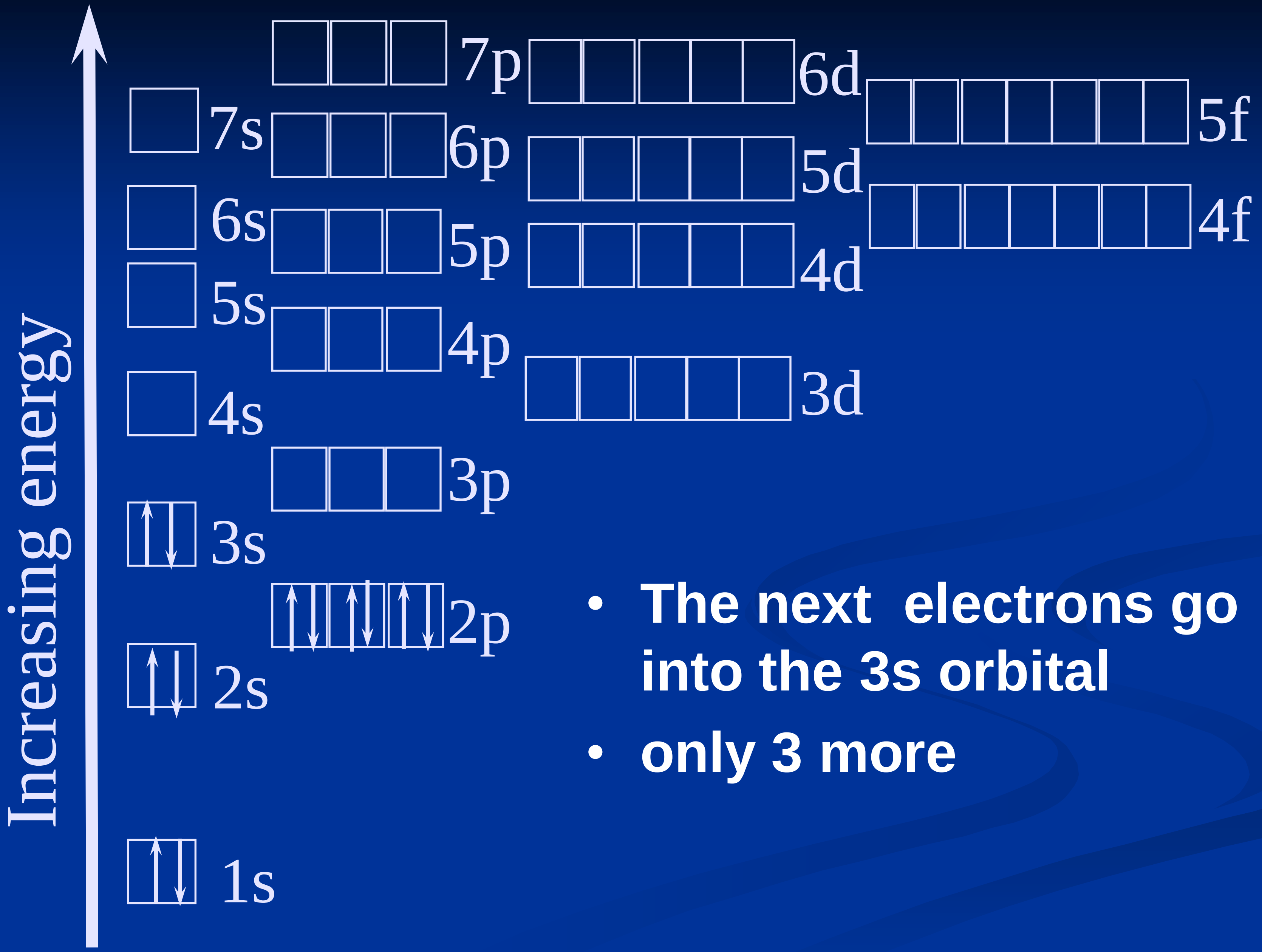
- only 13 more to go



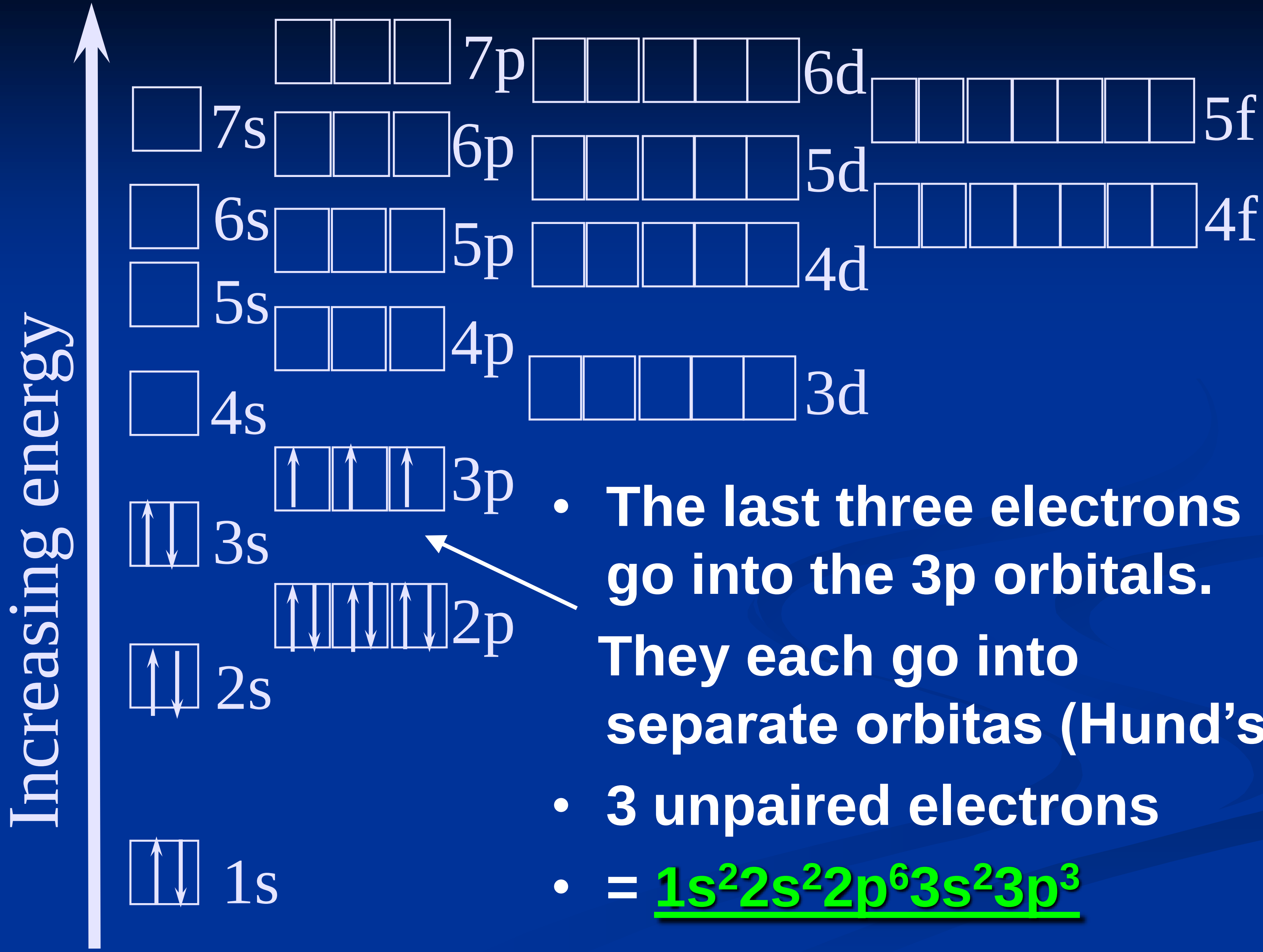
- The next electrons go into the 2s orbital
- only 11 more



- **The next electrons go into the 2p orbital**
- **only 5 more**



- **The next electrons go into the 3s orbital**
- **only 3 more**



- The last three electrons go into the 3p orbitals.

  They each go into separate orbitas (Hund's)
- 3 unpaired electrons
- = $1s^22s^22p^63s^23p^3$

Practice Electron Configuration and Orbital Notation

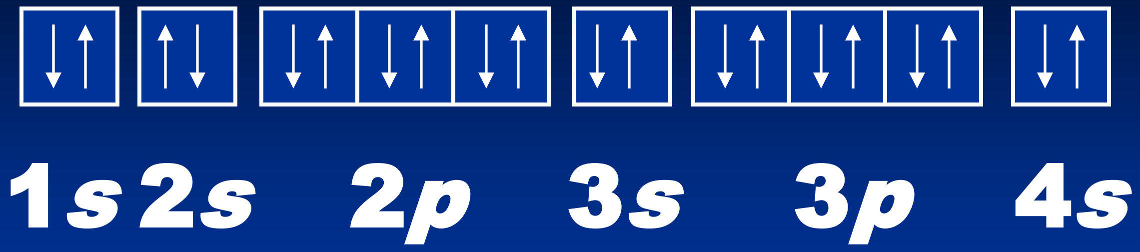
Write the electron configuration and orbital notation for each of the following

$Z = 20$

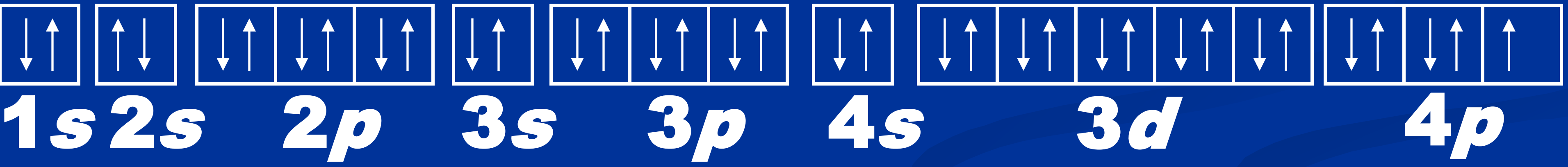
$Z = 35$

$Z = 26$

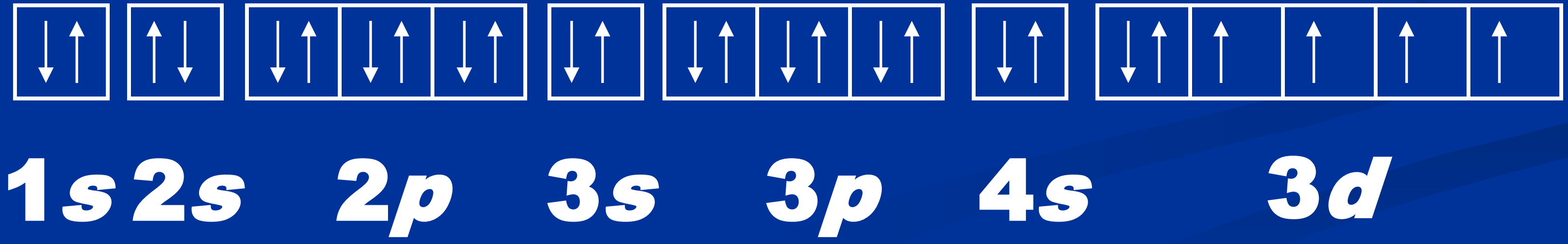
$Z = 20$ $1s^22s^22p^63s^23p^64s^2$ **(Ca)**



$Z = 35$ $1s^22s^22p^63s^23p^64s^23d^{10}4p^5$ **(Br)**

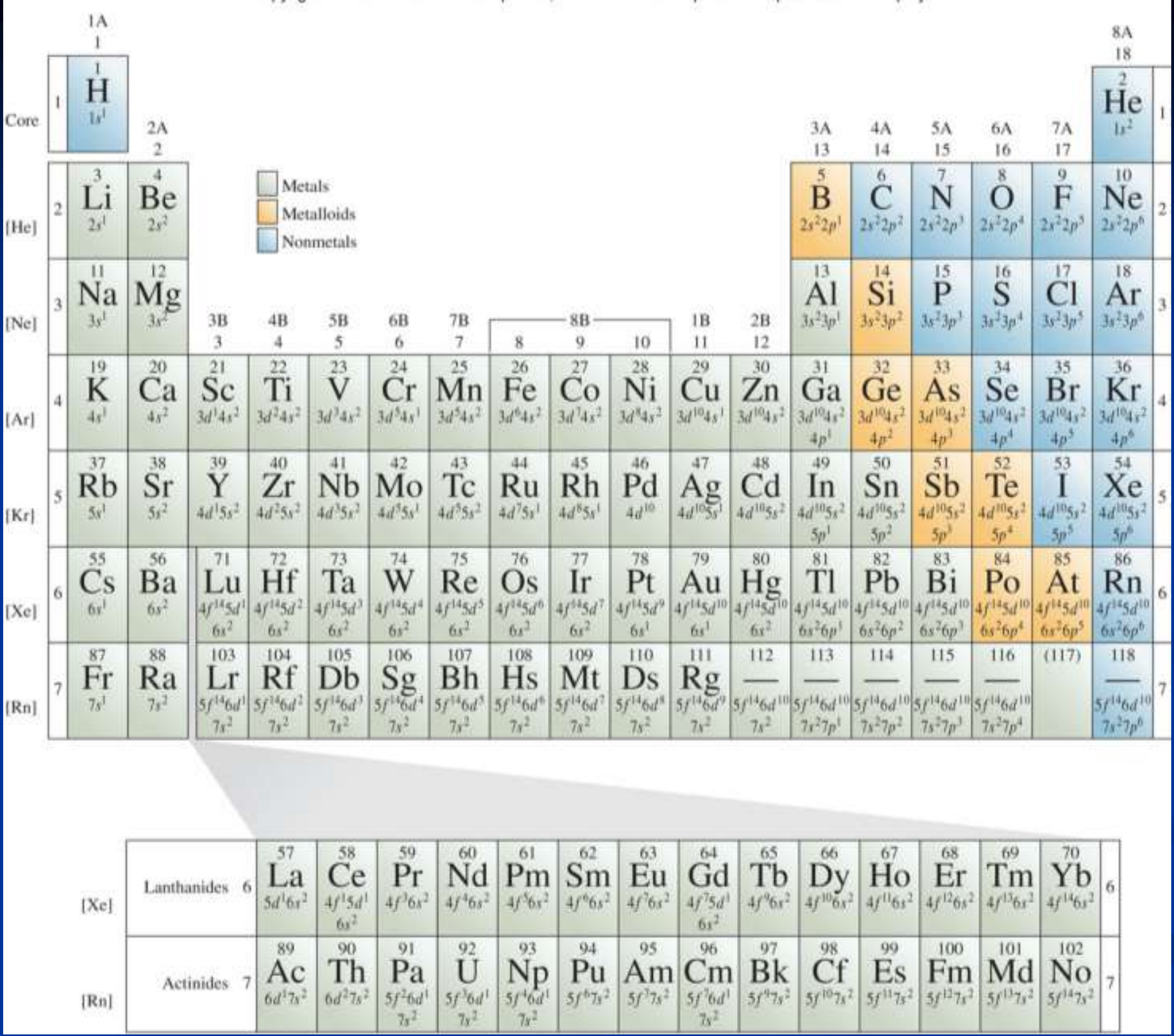


$Z = 26$ $1s^22s^22p^63s^23p^64s^23d^6$ **(Fe)**



6.9 Electron Configurations and the Periodic Table

- Position on the periodic table indicates electron configuration
- What similarities are found within groups on the table?

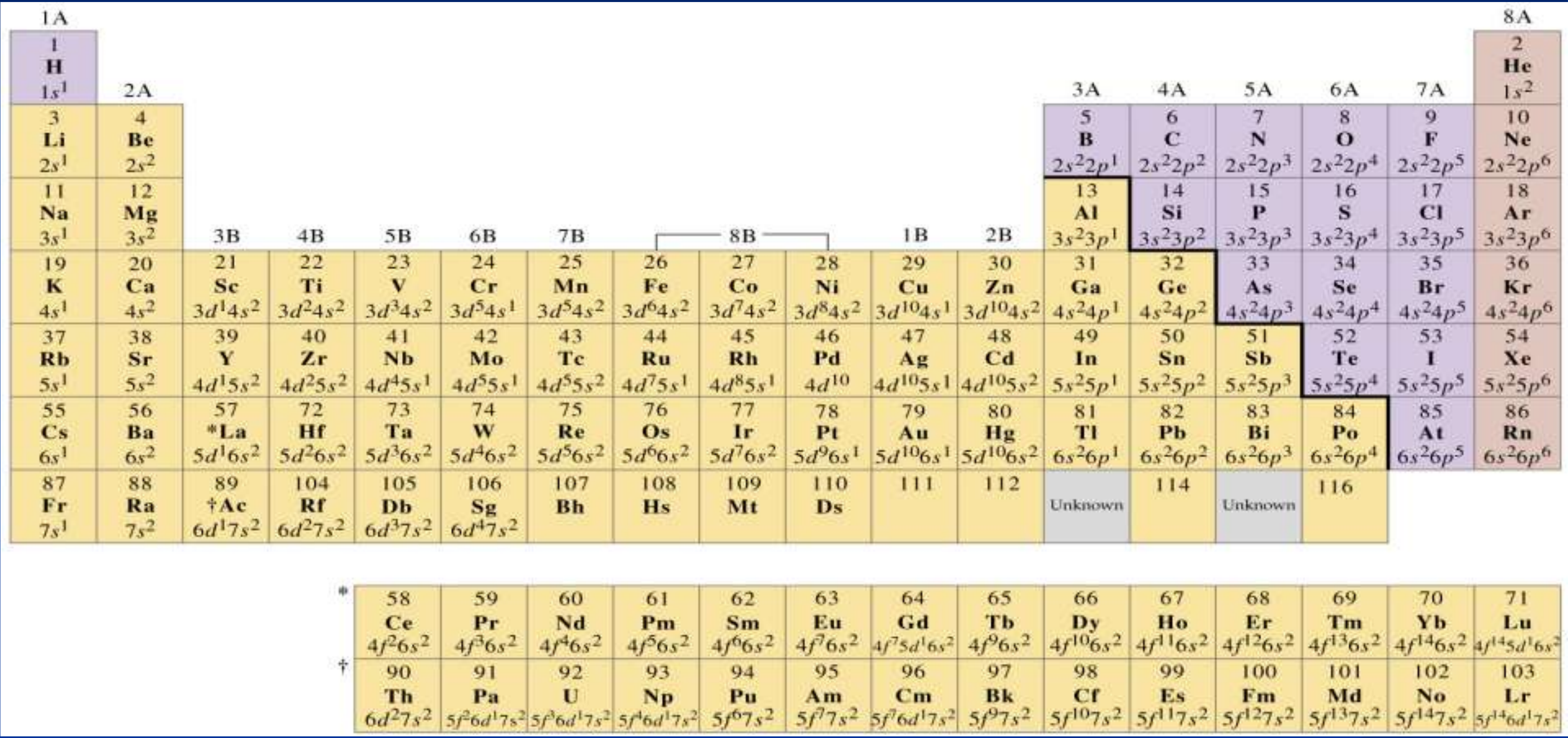


Metals
Metalloids
Nonmetals

Core		1A 1	2A 2	3B 3	4B 4	5B 5	6B 6	7B 7	8B 8	9	10	1B 11	2B 12	3A 13	4A 14	5A 15	6A 16	7A 17	8A 18	
	1	1 H $1s^{1}$																	2 He $1s^{2}$	1
[He]	2	3 Li $2s^{1}$	4 Be $2s^{2}$											5 B $2s^{2}2p^{1}$	6 C $2s^{2}2p^{2}$	7 N $2s^{2}2p^{3}$	8 O $2s^{2}2p^{4}$	9 F $2s^{2}2p^{5}$	10 Ne $2s^{2}2p^{6}$	2
[Ne]	3	11 Na $3s^{1}$	12 Mg $3s^{2}$											13 Al $3s^{2}3p^{1}$	14 Si $3s^{2}3p^{2}$	15 P $3s^{2}3p^{3}$	16 S $3s^{2}3p^{4}$	17 Cl $3s^{2}3p^{5}$	18 Ar $3s^{2}3p^{6}$	3
[Ar]	4	19 K $4s^{1}$	20 Ca $4s^{2}$	21 Sc $3d^{1}4s^{2}$	22 Ti $3d^{2}4s^{2}$	23 V $3d^{3}4s^{2}$	24 Cr $3d^{5}4s^{1}$	25 Mn $3d^{5}4s^{2}$	26 Fe $3d^{6}4s^{2}$	27 Co $3d^{7}4s^{2}$	28 Ni $3d^{8}4s^{2}$	29 Cu $3d^{10}4s^{1}$	30 Zn $3d^{10}4s^{2}$	31 Ga $3d^{10}4s^{2}4p^{1}$	32 Ge $3d^{10}4s^{2}4p^{2}$	33 As $3d^{10}4s^{2}4p^{3}$	34 Se $3d^{10}4s^{2}4p^{4}$	35 Br $3d^{10}4s^{2}4p^{5}$	36 Kr $3d^{10}4s^{2}4p^{6}$	4
[Kr]	5	37 Rb $5s^{1}$	38 Sr $5s^{2}$	39 Y $4d^{1}5s^{2}$	40 Zr $4d^{2}5s^{2}$	41 Nb $4d^{3}5s^{2}$	42 Mo $4d^{5}5s^{1}$	43 Tc $4d^{5}5s^{2}$	44 Ru $4d^{7}5s^{1}$	45 Rh $4d^{8}5s^{1}$	46 Pd $4d^{10}$	47 Ag $4d^{10}5s^{1}$	48 Cd $4d^{10}5s^{2}$	49 In $4d^{10}5s^{2}5p^{1}$	50 Sn $4d^{10}5s^{2}5p^{2}$	51 Sb $4d^{10}5s^{2}5p^{3}$	52 Te $4d^{10}5s^{2}5p^{4}$	53 I $4d^{10}5s^{2}5p^{5}$	54 Xe $4d^{10}5s^{2}5p^{6}$	5
[Xe]	6	55 Cs $6s^{1}$	56 Ba $6s^{2}$	71 Lu $4f^{14}5d^{1}6s^{2}$	72 Hf $4f^{14}5d^{2}6s^{2}$	73 Ta $4f^{14}5d^{3}6s^{2}$	74 W $4f^{14}5d^{4}6s^{2}$	75 Re $4f^{14}5d^{5}6s^{2}$	76 Os $4f^{14}5d^{6}6s^{2}$	77 Ir $4f^{14}5d^{7}6s^{2}$	78 Pt $4f^{14}5d^{9}6s^{1}$	79 Au $4f^{14}5d^{10}6s^{1}$	80 Hg $4f^{14}5d^{10}6s^{2}$	81 Tl $4f^{14}5d^{10}6s^{2}6p^{1}$	82 Pb $4f^{14}5d^{10}6s^{2}6p^{2}$	83 Bi $4f^{14}5d^{10}6s^{2}6p^{3}$	84 Po $4f^{14}5d^{10}6s^{2}6p^{4}$	85 At $4f^{14}5d^{10}6s^{2}6p^{5}$	86 Rn $4f^{14}5d^{10}6s^{2}6p^{6}$	6
[Rn]	7	87 Fr $7s^{1}$	88 Ra $7s^{2}$	103 Lr $5f^{14}6d^{1}7s^{2}$	104 Rf $5f^{14}6d^{2}7s^{2}$	105 Db $5f^{14}6d^{3}7s^{2}$	106 Sg $5f^{14}6d^{4}7s^{2}$	107 Bh $5f^{14}6d^{5}7s^{2}$	108 Hs $5f^{14}6d^{6}7s^{2}$	109 Mt $5f^{14}6d^{7}7s^{2}$	110 Ds $5f^{14}6d^{8}7s^{2}$	111 Rg $5f^{14}6d^{9}7s^{2}$	112 — $5f^{14}6d^{10}7s^{2}$	113 — $5f^{14}6d^{10}7s^{2}7p^{1}$	114 — $5f^{14}6d^{10}7s^{2}7p^{2}$	115 — $5f^{14}6d^{10}7s^{2}7p^{3}$	116 — $5f^{14}6d^{10}7s^{2}7p^{4}$	(117)	118 — $5f^{14}6d^{10}7s^{2}7p^{6}$	7

[Xe]	Lanthanides	6	57 La $5d^{1}6s^{2}$	58 Ce $4f^{1}5d^{1}6s^{2}$	59 Pr $4f^{3}6s^{2}$	60 Nd $4f^{4}6s^{2}$	61 Pm $4f^{5}6s^{2}$	62 Sm $4f^{6}6s^{2}$	63 Eu $4f^{7}6s^{2}$	64 Gd $4f^{7}5d^{1}6s^{2}$	65 Tb $4f^{9}6s^{2}$	66 Dy $4f^{10}6s^{2}$	67 Ho $4f^{11}6s^{2}$	68 Er $4f^{12}6s^{2}$	69 Tm $4f^{13}6s^{2}$	70 Yb $4f^{14}6s^{2}$	6
[Rn]	Actinides	7	89 Ac $6d^{1}7s^{2}$	90 Th $6d^{2}7s^{2}$	91 Pa $5f^{2}6d^{1}7s^{2}$	92 U $5f^{3}6d^{1}7s^{2}$	93 Np $5f^{4}6d^{1}7s^{2}$	94 Pu $5f^{6}7s^{2}$	95 Am $5f^{7}7s^{2}$	96 Cm $5f^{7}6d^{1}7s^{2}$	97 Bk $5f^{9}7s^{2}$	98 Cf $5f^{10}7s^{2}$	99 Es $5f^{11}7s^{2}$	100 Fm $5f^{12}7s^{2}$	101 Md $5f^{13}7s^{2}$	102 No $5f^{14}7s^{2}$	7

Periodic Relationships



1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A	8A
1 **H** $1s^{1}$																	2 **He** $1s^{2}$
3 **Li** $2s^{1}$	4 **Be** $2s^{2}$											5 **B** $2s^{2}2p^{1}$	6 **C** $2s^{2}2p^{2}$	7 **N** $2s^{2}2p^{3}$	8 **O** $2s^{2}2p^{4}$	9 **F** $2s^{2}2p^{5}$	10 **Ne** $2s^{2}2p^{6}$
11 **Na** $3s^{1}$	12 **Mg** $3s^{2}$											13 **Al** $3s^{2}3p^{1}$	14 **Si** $3s^{2}3p^{2}$	15 **P** $3s^{2}3p^{3}$	16 **S** $3s^{2}3p^{4}$	17 **Cl** $3s^{2}3p^{5}$	18 **Ar** $3s^{2}3p^{6}$
19 **K** $4s^{1}$	20 **Ca** $4s^{2}$	21 **Sc** $3d^{1}4s^{2}$	22 **Ti** $3d^{2}4s^{2}$	23 **V** $3d^{3}4s^{2}$	24 **Cr** $3d^{5}4s^{1}$	25 **Mn** $3d^{5}4s^{2}$	26 **Fe** $3d^{6}4s^{2}$	27 **Co** $3d^{7}4s^{2}$	28 **Ni** $3d^{8}4s^{2}$	29 **Cu** $3d^{10}4s^{1}$	30 **Zn** $3d^{10}4s^{2}$	31 **Ga** $4s^{2}4p^{1}$	32 **Ge** $4s^{2}4p^{2}$	33 **As** $4s^{2}4p^{3}$	34 **Se** $4s^{2}4p^{4}$	35 **Br** $4s^{2}4p^{5}$	36 **Kr** $4s^{2}4p^{6}$
37 **Rb** $5s^{1}$	38 **Sr** $5s^{2}$	39 **Y** $4d^{1}5s^{2}$	40 **Zr** $4d^{2}5s^{2}$	41 **Nb** $4d^{4}5s^{1}$	42 **Mo** $4d^{5}5s^{1}$	43 **Tc** $4d^{5}5s^{2}$	44 **Ru** $4d^{7}5s^{1}$	45 **Rh** $4d^{8}5s^{1}$	46 **Pd** $4d^{10}$	47 **Ag** $4d^{10}5s^{1}$	48 **Cd** $4d^{10}5s^{2}$	49 **In** $5s^{2}5p^{1}$	50 **Sn** $5s^{2}5p^{2}$	51 **Sb** $5s^{2}5p^{3}$	52 **Te** $5s^{2}5p^{4}$	53 **I** $5s^{2}5p^{5}$	54 **Xe** $5s^{2}5p^{6}$
55 **Cs** $6s^{1}$	56 **Ba** $6s^{2}$	57 ***La** $5d^{1}6s^{2}$	72 **Hf** $5d^{2}6s^{2}$	73 **Ta** $5d^{3}6s^{2}$	74 **W** $5d^{4}6s^{2}$	75 **Re** $5d^{5}6s^{2}$	76 **Os** $5d^{6}6s^{2}$	77 **Ir** $5d^{7}6s^{2}$	78 **Pt** $5d^{9}6s^{1}$	79 **Au** $5d^{10}6s^{1}$	80 **Hg** $5d^{10}6s^{2}$	81 **Tl** $6s^{2}6p^{1}$	82 **Pb** $6s^{2}6p^{2}$	83 **Bi** $6s^{2}6p^{3}$	84 **Po** $6s^{2}6p^{4}$	85 **At** $6s^{2}6p^{5}$	86 **Rn** $6s^{2}6p^{6}$
87 **Fr** $7s^{1}$	88 **Ra** $7s^{2}$	89 **†Ac** $6d^{1}7s^{2}$	104 **Rf** $6d^{2}7s^{2}$	105 **Db** $6d^{3}7s^{2}$	106 **Sg** $6d^{4}7s^{2}$	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111	112	Unknown	114	Unknown	116		
			*	58 **Ce** $4f^{2}6s^{2}$	59 **Pr** $4f^{3}6s^{2}$	60 **Nd** $4f^{4}6s^{2}$	61 **Pm** $4f^{5}6s^{2}$	62 **Sm** $4f^{6}6s^{2}$	63 **Eu** $4f^{7}6s^{2}$	64 **Gd** $4f^{7}5d^{1}6s^{2}$	65 **Tb** $4f^{9}6s^{2}$	66 **Dy** $4f^{10}6s^{2}$	67 **Ho** $4f^{11}6s^{2}$	68 **Er** $4f^{12}6s^{2}$	69 **Tm** $4f^{13}6s^{2}$	70 **Yb** $4f^{14}6s^{2}$	71 **Lu** $4f^{14}5d^{1}6s^{2}$
			†	90 **Th** $6d^{2}7s^{2}$	91 **Pa** $5f^{2}6d^{1}7s^{2}$	92 **U** $5f^{3}6d^{1}7s^{2}$	93 **Np** $5f^{4}6d^{1}7s^{2}$	94 **Pu** $5f^{6}7s^{2}$	95 **Am** $5f^{7}7s^{2}$	96 **Cm** $5f^{7}6d^{1}7s^{2}$	97 **Bk** $5f^{9}7s^{2}$	98 **Cf** $5f^{10}7s^{2}$	99 **Es** $5f^{11}7s^{2}$	100 **Fm** $5f^{12}7s^{2}$	101 **Md** $5f^{13}7s^{2}$	102 **No** $5f^{14}7s^{2}$	103 **Lr** $5f^{14}6d^{1}7s^{2}$

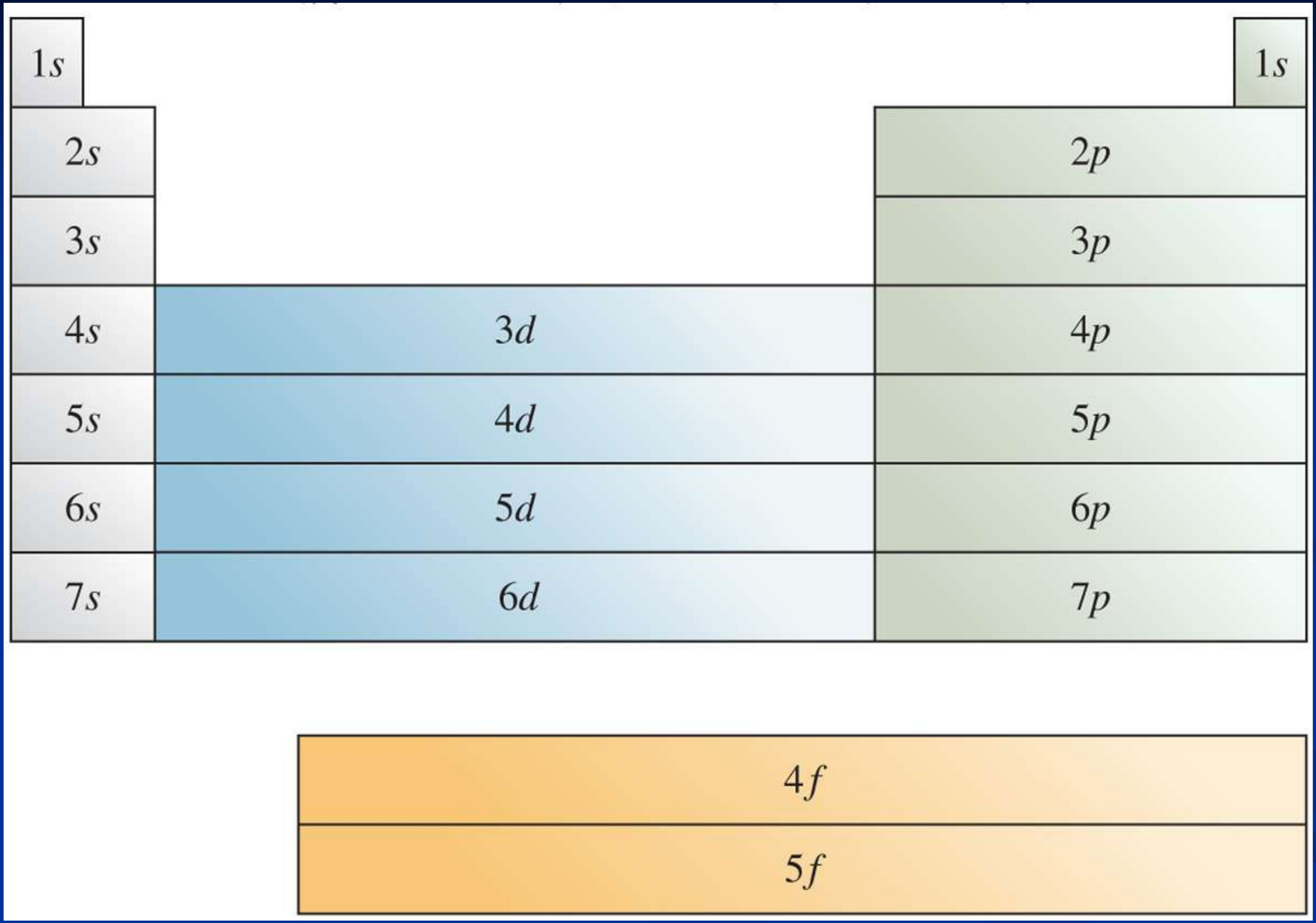
Electron Configurations and the Periodic Table

- *Noble gas core configuration* - can be used to represent all elements but H and He

Example:

$Z = 15$ $[1s^2 2s^2 2p^6] 3s^2 3p^3$ (P)

$[\text{Ne}]\ 3s^2 3p^3$ (P)


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

Exceptions to the aufbau rule

- Not all elements follow the “order” of the diagonal rule
- Notable exceptions: Cu ($Z = 29$) and Cr ($Z = 24$)

$$\text{Cu} = [\text{Ar}]4s^1 3d^{10}$$

$$\text{Cr} = [\text{Ar}]4s^1 3d^5$$

Reason: slightly greater stability associated with filled and half-filled *d* subshells

Key Points

- Electromagnetic spectrum
- Wavelength, frequency, energy (calculate)
- Quanta (of light - photon)
- Photoelectric effect
- Emission spectra
- Ground state vs excited state
- Heisenberg uncertainty principle

Key Points

- Quantum numbers (n, l, m_l, m_s) predict values and possible sets
- Electron configuration - identify and write (also noble gas core)
- Pauli exclusion principle, Hund's rule, Aufbau principle