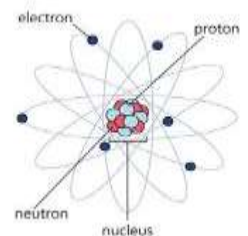


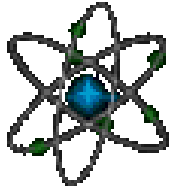


# CHAPTER 2

## ATOMIC STRUCTURE

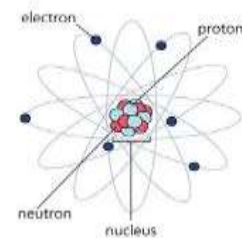
- **2.1 Bohr's atomic model**
- **2.2 Quantum mechanics**
- **2.3 Electronic configuration**





# 2.1

## BOHR'S ATOMIC MODEL





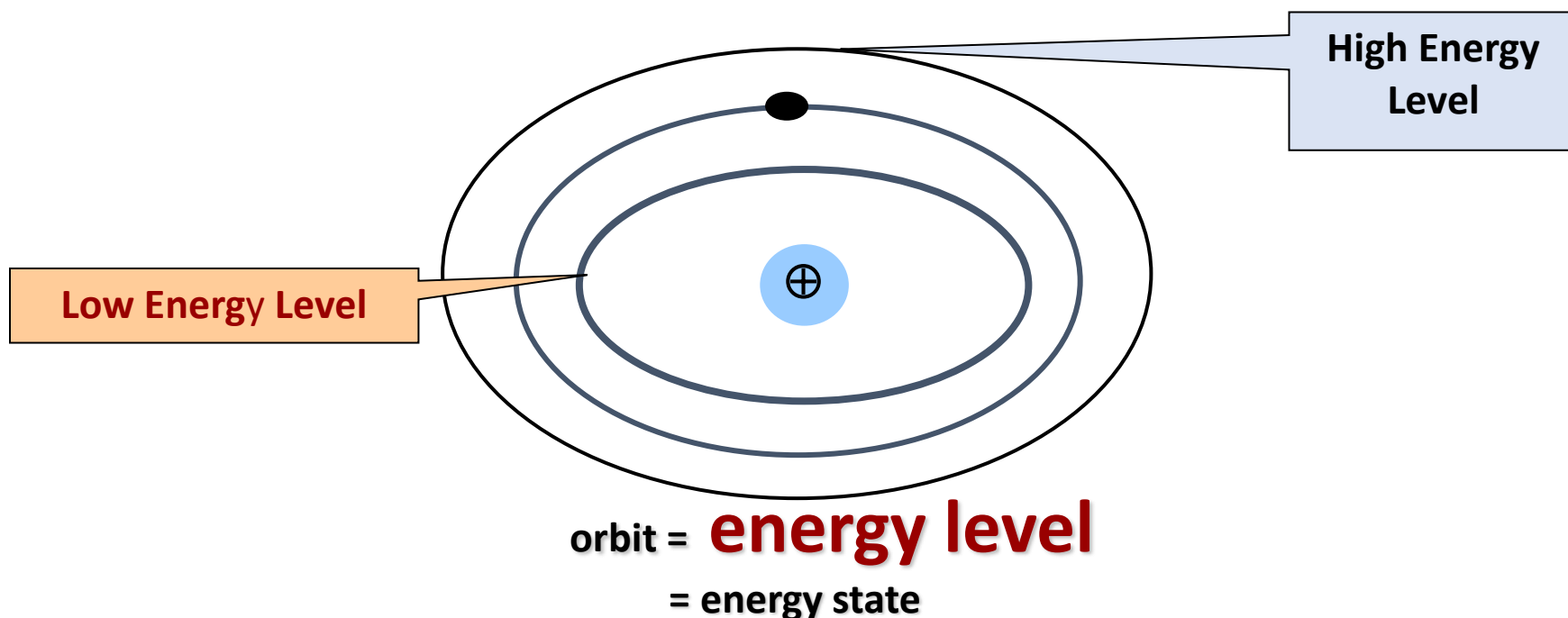
# Bohr's Atomic Model

Four Bohr's atomic postulate:

1

Electron moves in circular orbit around the nucleus of an atom

- electron does **not release or absorb** any energy at stationary state.



2

In the specific **energy level**, the energy of electron is **fixed in value or is quantised**.

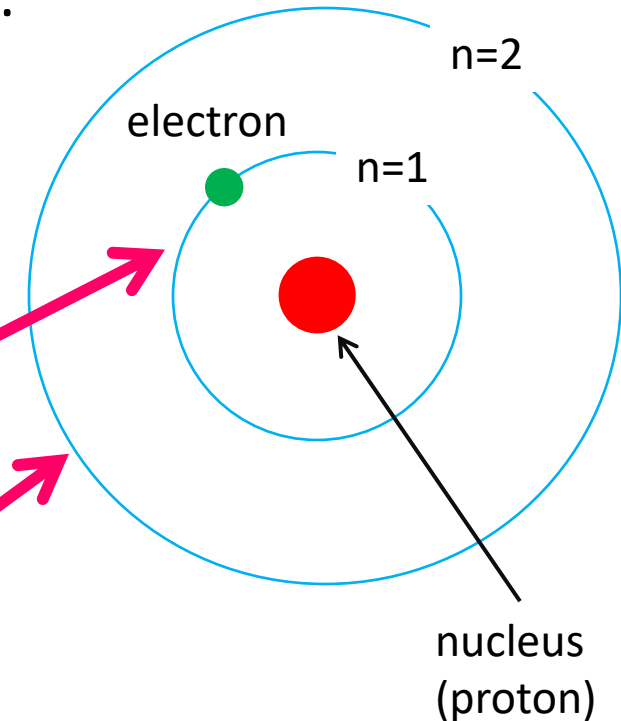
(quantised = fixed/specific/definite)

This means that an electron moving in an orbit can have a certain amount of energy.

$$E_n = -R_H \left( \frac{1}{n^2} \right)$$

$$E_1 = -R_H \left( \frac{1}{1^2} \right)$$

$$E_2 = -R_H \left( \frac{1}{2^2} \right)$$



**$n$ : Principal quantum number/ energy level= 1, 2, 3, ..... $\infty$**

3

❑ An electron **moves in an allowed energy state** will **not absorb or radiate** energy.

☞ **no change of energy** while electron moves within an orbit

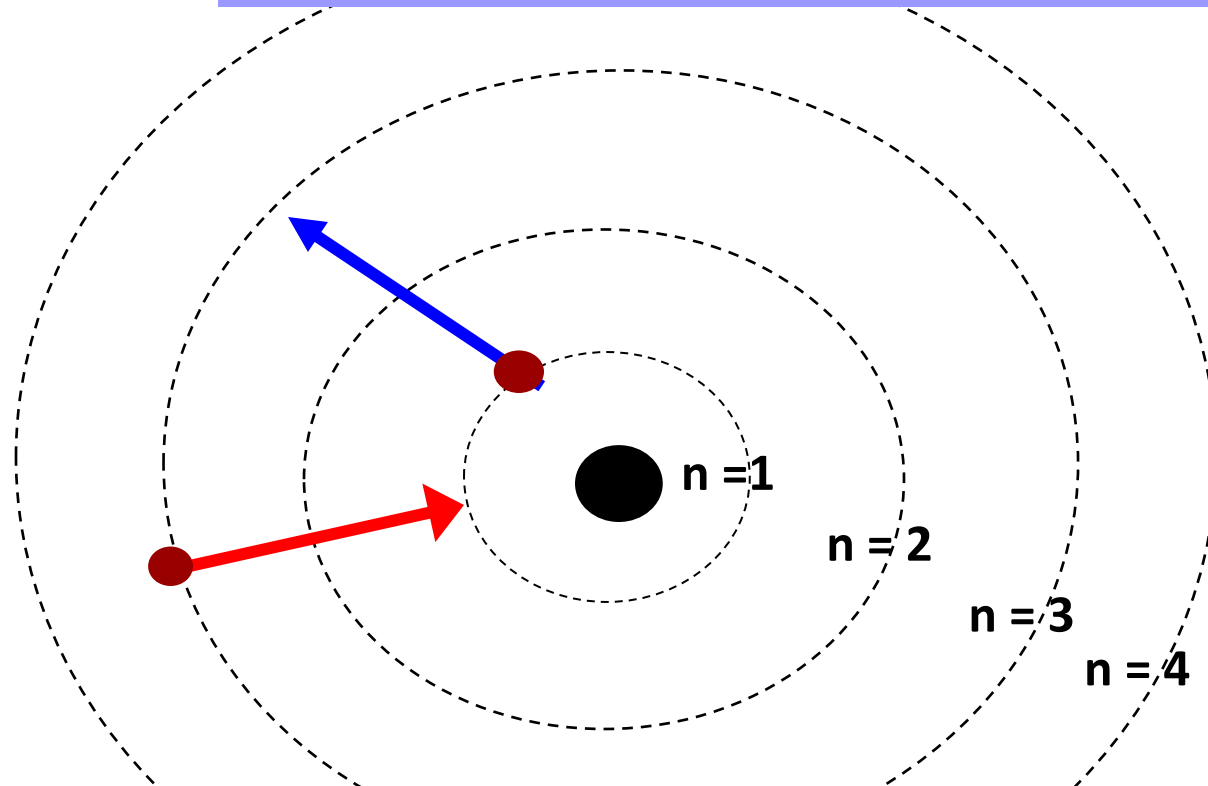
4

❑ Energy is **emitted or absorbed** by an electron as it **changes from one allowed energy state to another.**

# The existence of electron energy levels in an atom

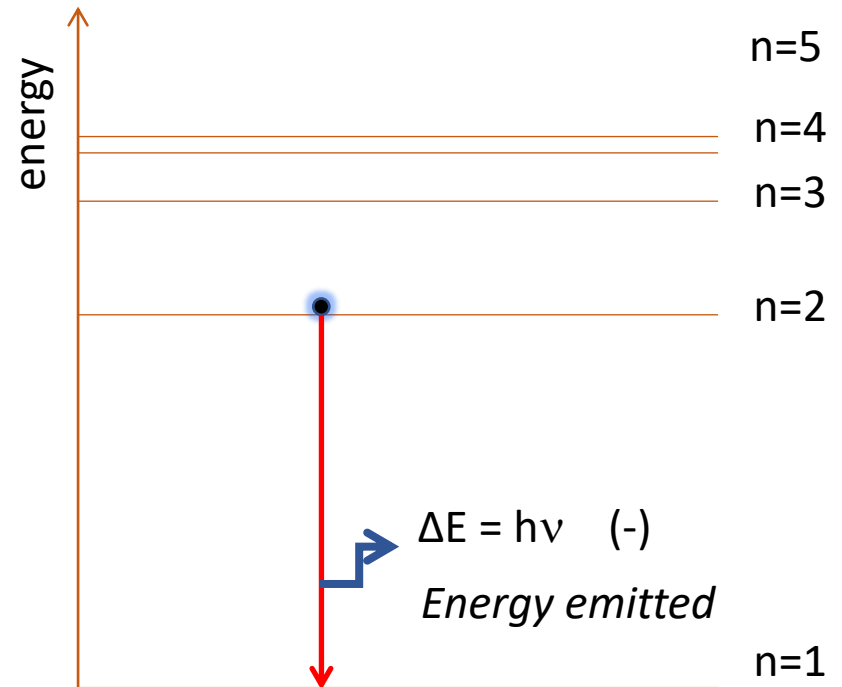
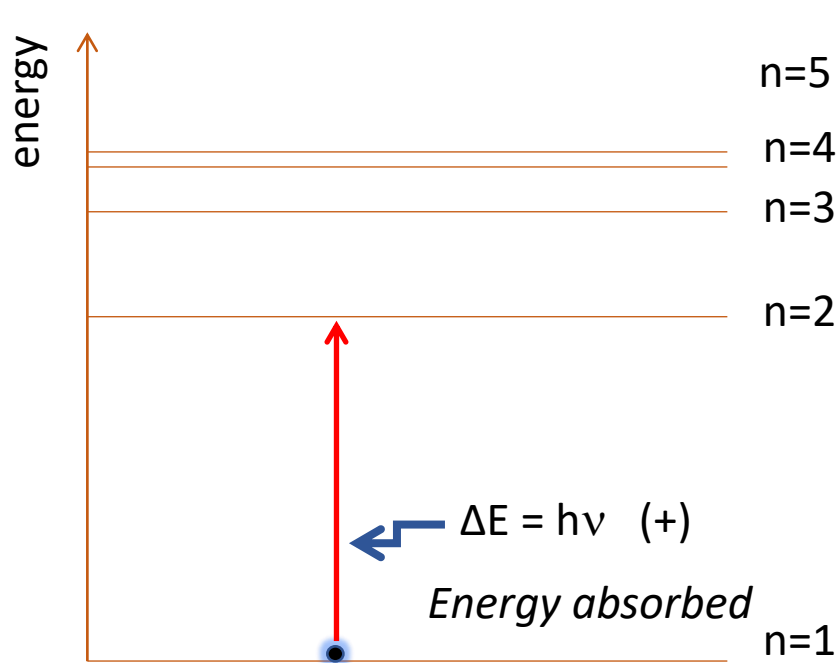
- The energy of an electron in an atom is quantised. This means that an electron moving in an orbit can have only a certain amount of energy.
- The electron nearest to the nucleus has the lowest energy. The further the electron from the nucleus, the higher its energy.

When electron is absorbed specific amount of energy, electron is excited from lower to higher energy level



Electron falls from higher to lower energy level .  
A photon of energy is released.

***Photon = a packet of light energy equals to  $h\nu$***



Energy is **absorbed** in  
when electron **moves**  
from **lower energy level**  
to a **higher energy level**;

energy is **released** in the  
form of photon when  
electron **falls back from a**  
**higher energy level to a**  
**lower energy level.**



## POINTS TO REMEMBER

### Energy level

 energy associated with a specific orbit or state

### Ground state

 The electrons have their lowest energy

### Excited state

 The electrons have shifted from a lower energy level to a higher energy level

# BOHR'S ATOMIC MODEL

**Energy** of an **electron** in its level (stationary state):

$$E_n = - R_H \left( \frac{1}{n^2} \right)$$

$$\begin{aligned} R_H &= \text{Rydberg constant} \\ &= 2.18 \times 10^{-18} \text{ J} \end{aligned}$$

$$\begin{aligned} n &= \text{Principal quantum number} \\ &= 1, 2, 3, \dots, \infty \end{aligned}$$

## EXAMPLE 1

**Calculate the energy (in J) of an electron when it occupies a level equivalent to the quantum number of  $n = 3$  and  $n = 4$ .**



Energy of an electron at  $n = 3$  ( $E_3$ ) :

$$\begin{aligned} E_3 &= -R_H \left( \frac{1}{n^2} \right) \\ &= -2.18 \times 10^{-18} \text{ J} \times \left( \frac{1}{3^2} \right) \\ &= -2.42 \times 10^{-19} \text{ J} \end{aligned}$$

Energy of an electron at  $n = 4$  ( $E_4$ ) :

$$\begin{aligned} E_4 &= -R_H \left( \frac{1}{n^2} \right) \\ &= -2.18 \times 10^{-18} \text{ J} \times \left( \frac{1}{4^2} \right) \\ &= -1.36 \times 10^{-19} \text{ J} \end{aligned}$$

Tip:

☞  $n$  decrease (more close to nucleus) , Energy,  $E$  more negative

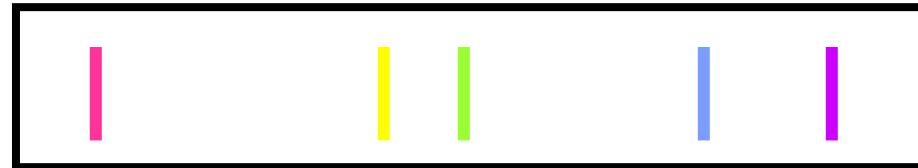
# TYPE OF SPECTRUM

SPECTRUM

Continuous Spectrum



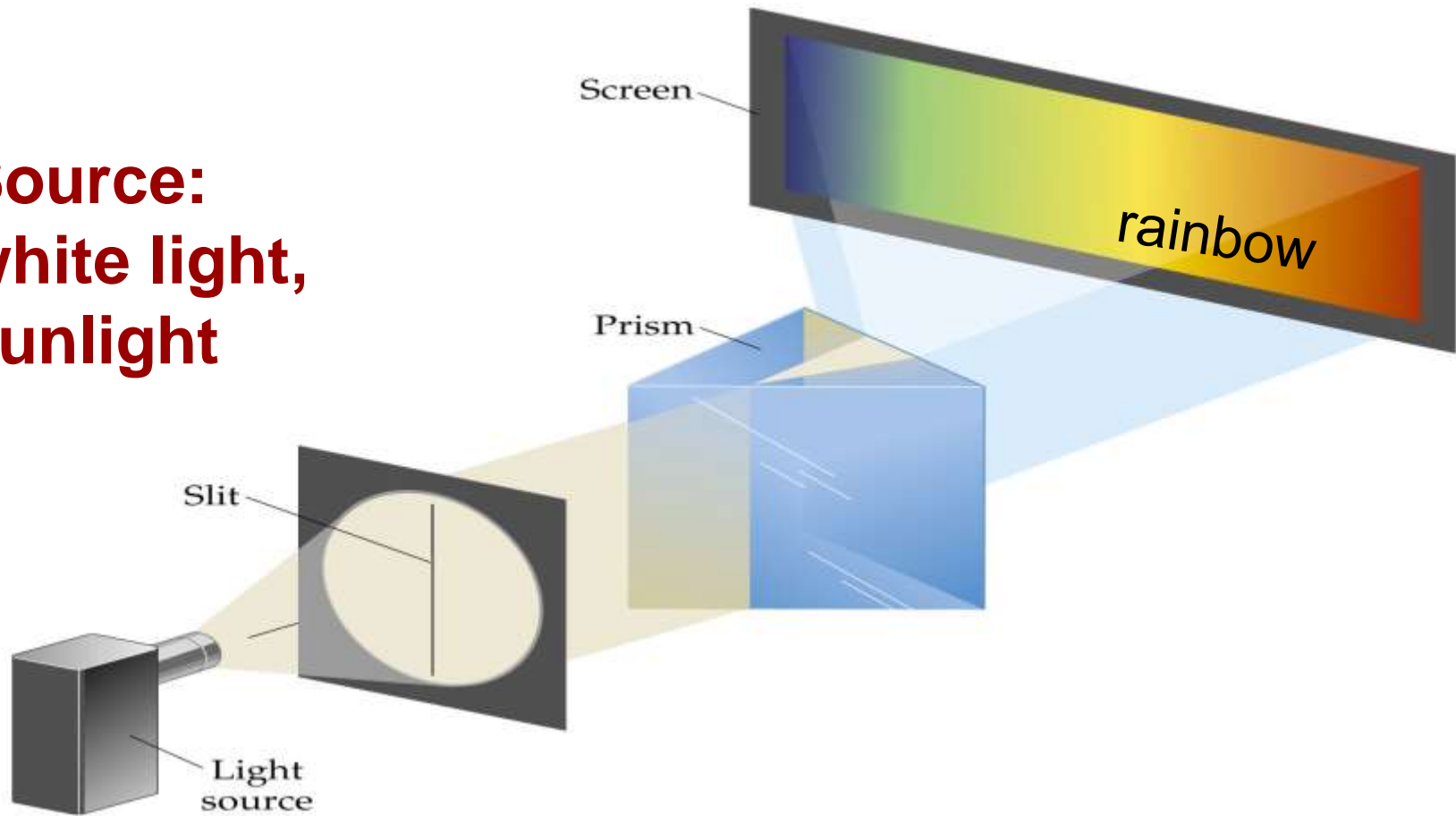
Line Spectrum



Hydrogen emission spectrum

# Continuous Spectrum

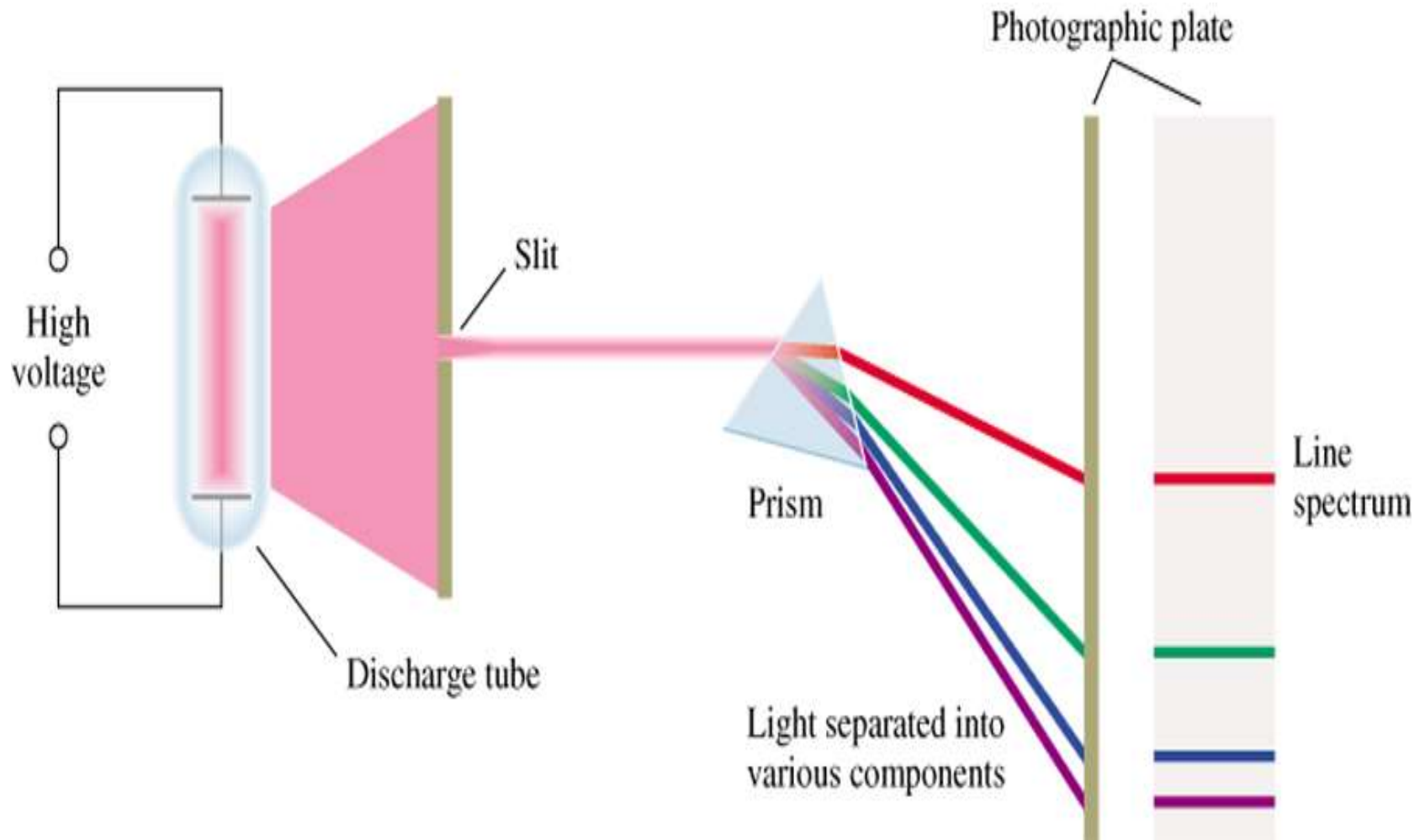
**Source:  
white light,  
sunlight**



❖ A spectrum that contains continuous band of light with all wavelengths.

# Line Spectrum

**Source: gas in discharge tube**



**A spectrum that contains a series of discrete lines separated by blank area and each line corresponds to specific wavelength.**

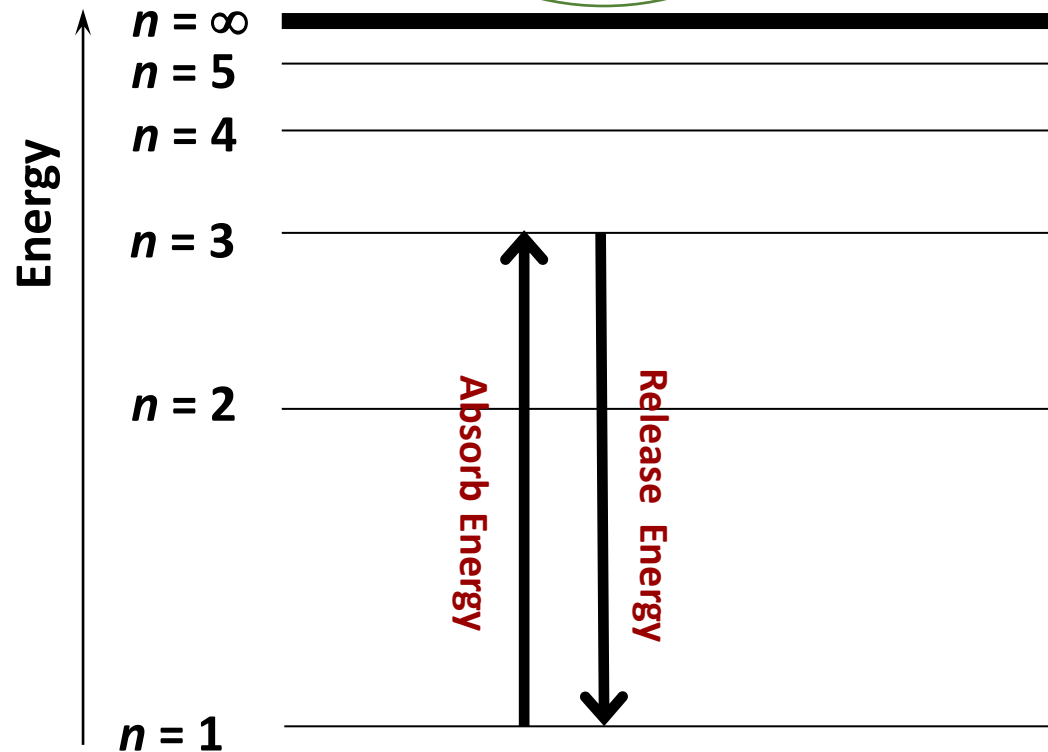
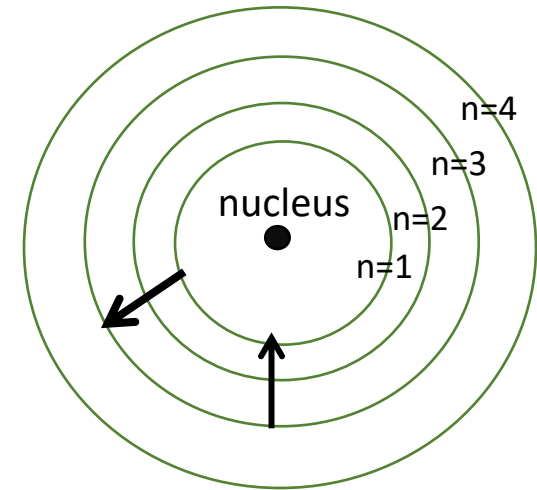
## How the line spectrum of hydrogen atom is formed?

When the electron of a hydrogen atom at its **ground state (lower energy level)** absorbs sufficient amount of energy, it will move to a **higher energy level**

At higher energy level, electron is **unstable**. It will fall back to a **lower energy level**.

During the transition (falls from higher to lower energy level), energy will be released in a form of **light (photon)** at definite **wavelength and frequency**.

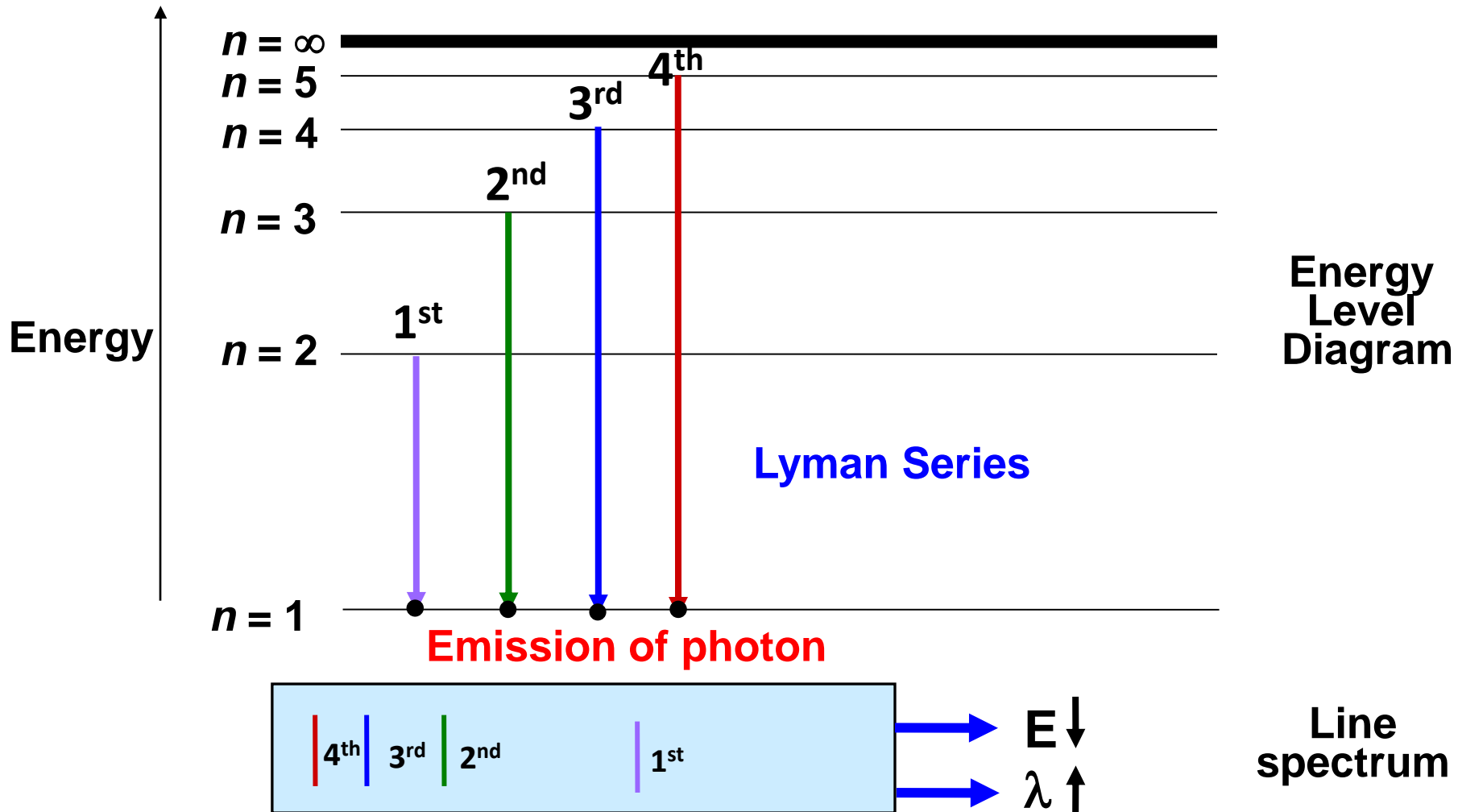
Since energy is quantised (fix in value), line spectrum is produced.



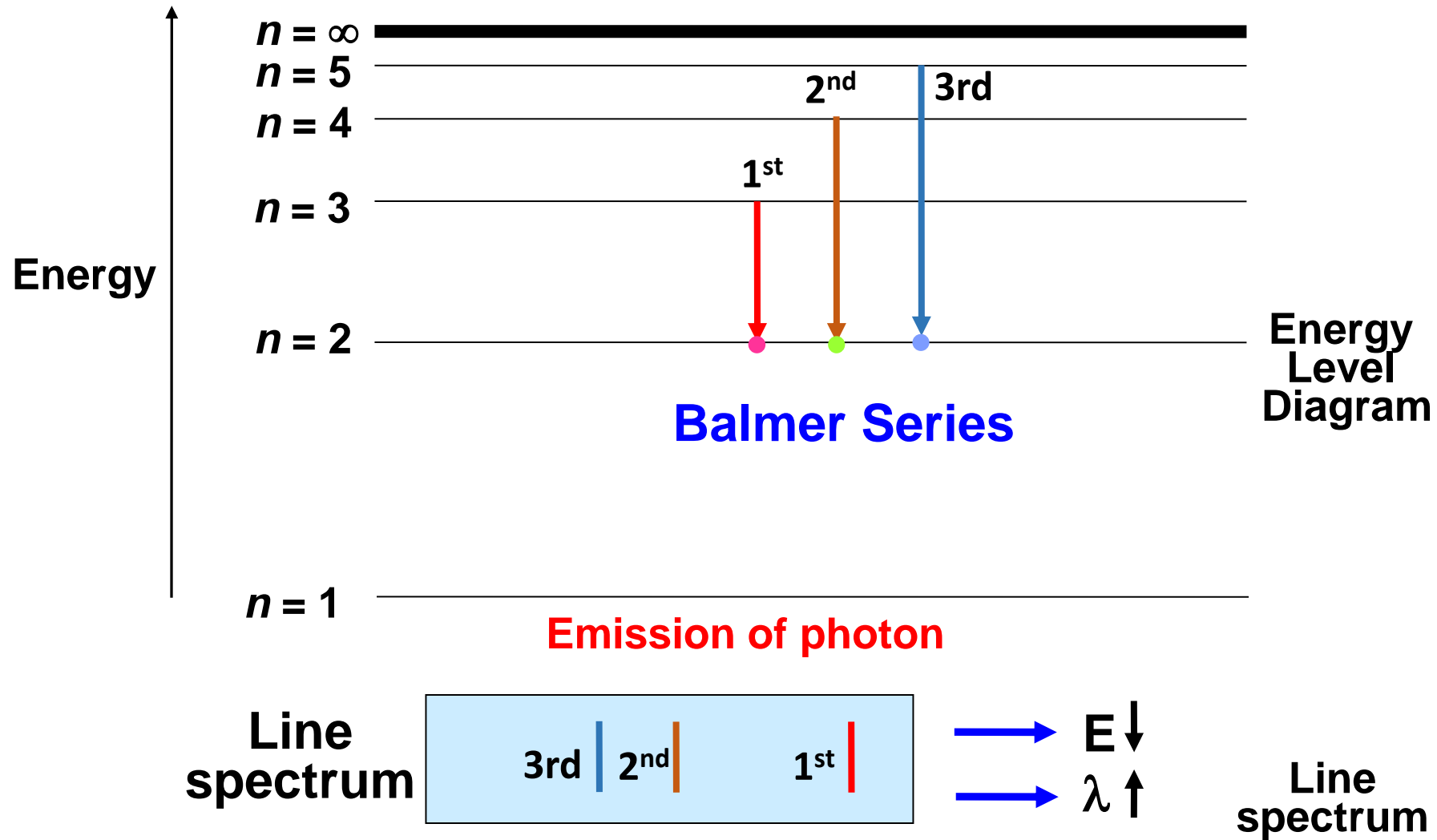


# FORMATION OF LINE SPECTRUM (emission series)

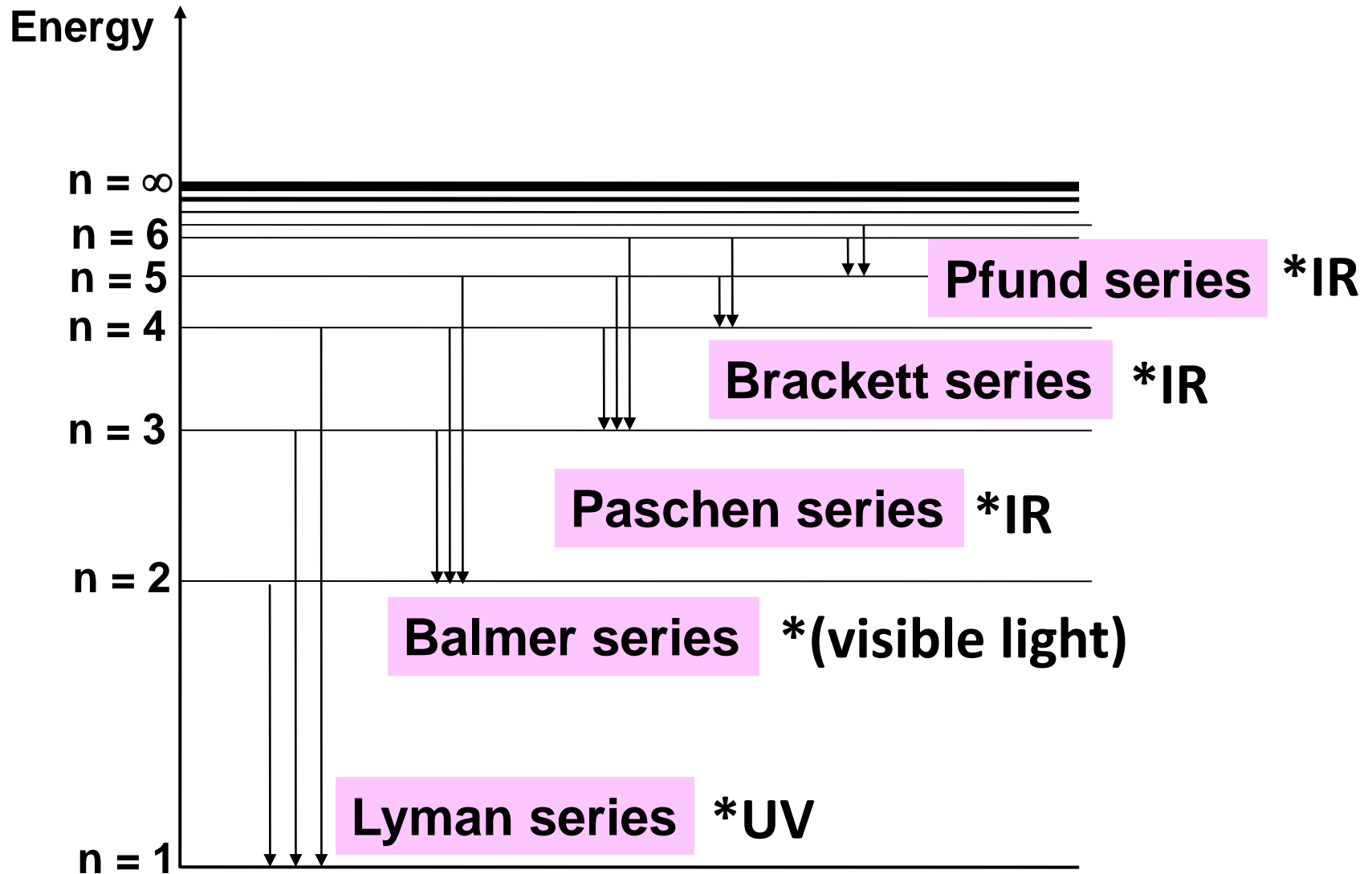
When the electrons fall back to lower energy levels, radiant energies (photons) are emitted in the form of light



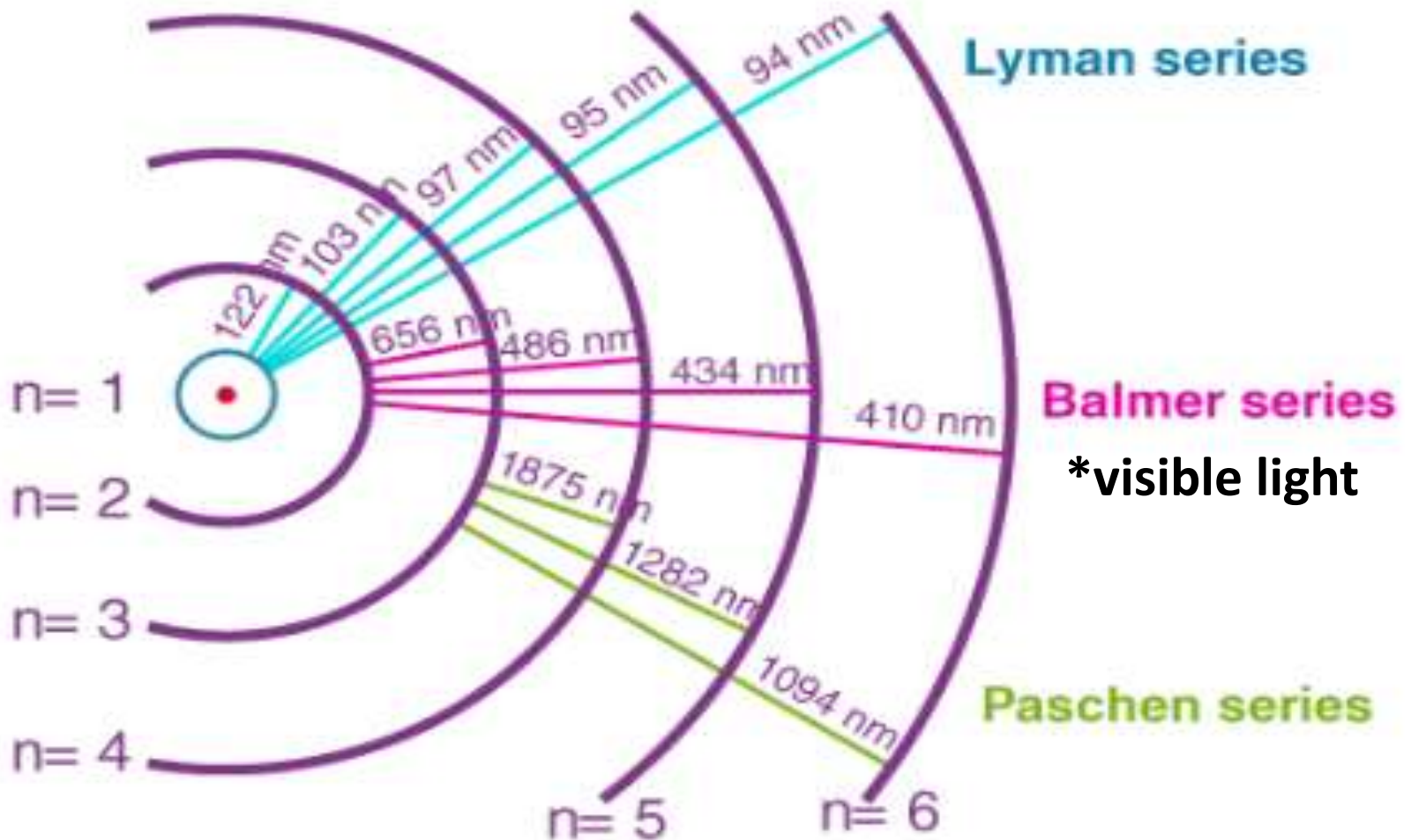
# FORMATION OF LINE SPECTRUM (emission series)



# Emission series of hydrogen atom



# Emission series of hydrogen atom (alternative diagram)



Source: <https://chem.libretexts.org>

# VARIOUS SERIES IN ATOMIC HYDROGEN EMISSION

Series	$n_f$	$n_i$	Spectrum region
<b>L</b> yman	1	2,3,4,...	ultraviolet
<b>B</b> almer	2	3,4,5,...	visible
<b>P</b> aschen	3	4,5,6,...	infrared
<b>B</b> rackett	4	5,6,7,...	infrared
<b>P</b> fund	5	6,7,8,...	infrared

**L**yman - **B**eli - **P**asu - **B**unga - **P**ecah

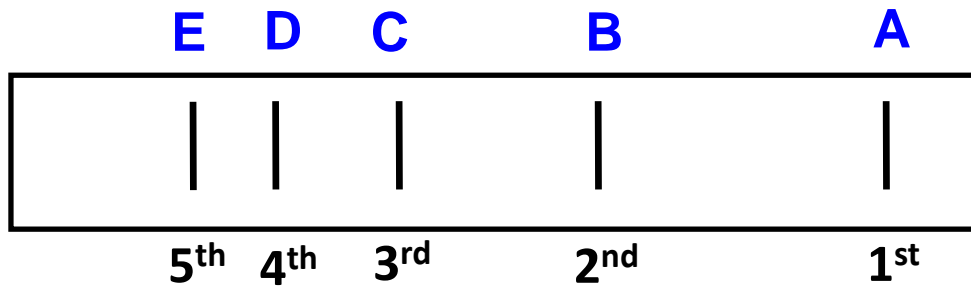
# Differences

Line spectrum	Continuous spectrum
A spectrum of radiation that consist of <b>discrete line</b> with <b>specific</b> wavelengths.	A spectrum that consists of <b>all wavelengths</b> in the visible region.
Each line is separated by blank area.	No blank area.
<b>Source:</b> light of discharge tube of $H_2$ , Na etc.	<b>Source:</b> white light, sun, moon etc.

## EXAMPLE 2

The following diagram represents the line spectrum of hydrogen atom for the Lyman series.

**Line spectrum**



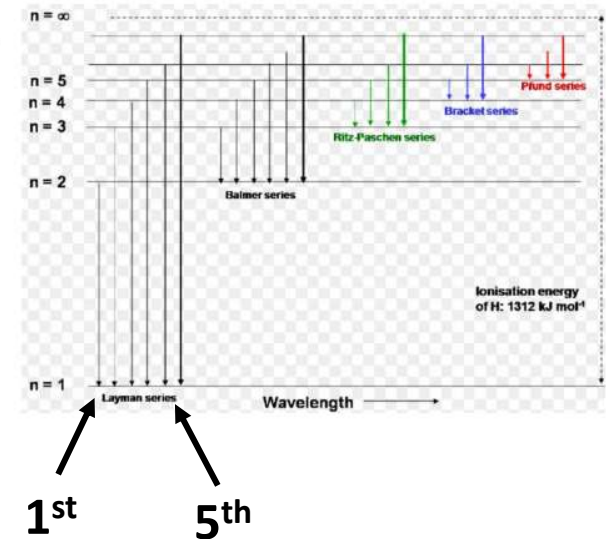
Specify the increasing order of the radiant energy, frequency and wavelength of the emitted photon.

Which of the line that corresponds to:

i. the fourth line? **Line D**

ii. the shortest wavelength? **Line E**

iii. the lowest frequency? **Line A**



# EXAMPLE 3

Line  
spectrum

Balmer series

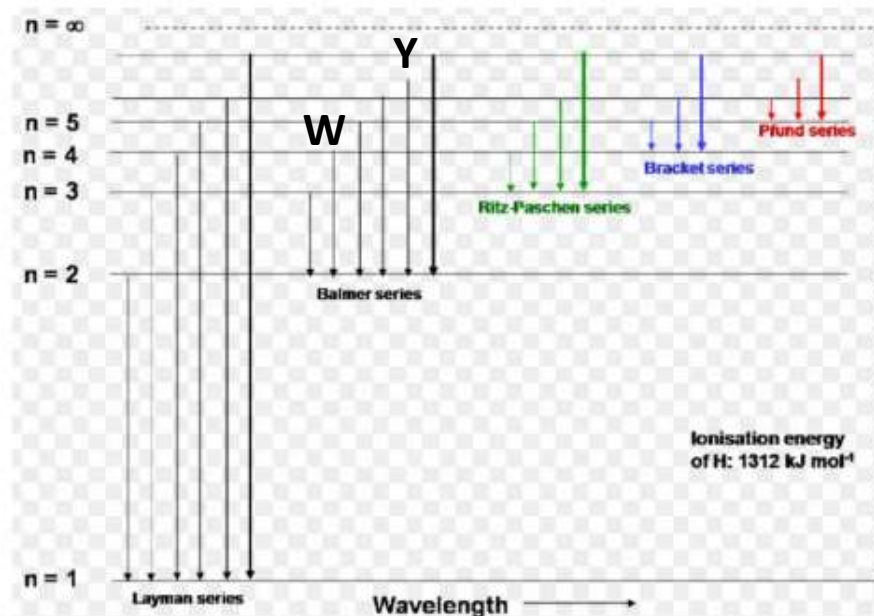
Y

W



Describe the transitions of electrons that lead to the lines W, and Y, respectively.

ANSWER:



For W: transition of electron from  $n=4$  to  $n=2$

For Y: transition of electron from  $n=7$  to  $n=2$



# BOHR'S ATOMIC MODEL

## ENERGY CHANGE ( $\Delta E$ )

$$E_1 = -R_H \left( \frac{1}{n_1^2} \right)$$

$$E_2 = -R_H \left( \frac{1}{n_2^2} \right)$$

$$\Delta E = E_2 - E_1$$

■ **Energy change** between any **two levels**:

$$\begin{aligned} \Delta E &= R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\ &= h\nu \end{aligned} \quad n_i = \text{initial}, n_f = \text{final}$$

# BOHR'S ATOMIC MODEL

- ☞ The amount of energy released by the electron during transition is called a **photon**
- ☞ A photon of energy is released in the **form of light** with appropriate **frequency and wavelength**.
- ☞ Therefore, the energy change (released/ absorbed) can be related as:

$$\Delta E = h\nu$$

$$c = \nu \times \lambda$$

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

$$\Delta E = \frac{hc}{\lambda}$$

$\lambda$  : wavelength (m)

$\nu$  : frequency

$c$  : speed of light =  $3.00 \times 10^8$  m/s

$h$  : Planck's constant =  $6.6256 \times 10^{-34}$  Js

## EXAMPLE 4

**Which of these electron transitions correspond to absorption of energy and which to emission?**

**a)  $n = 2$  to  $n = 4$**

**b)  $n = 3$  to  $n = 1$**



a)  $n = 2$  to  $n = 4$  ↑

☞ Electron transition: lower to higher level

☞ Absorption

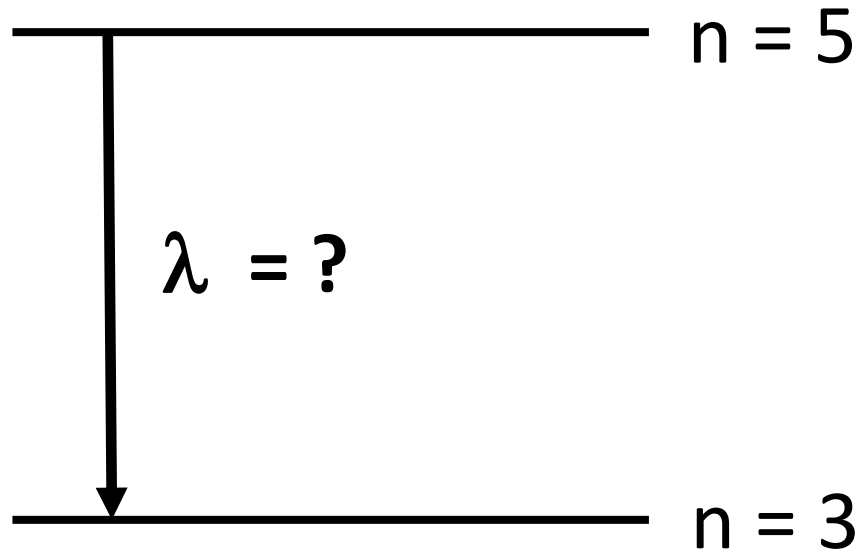
b)  $n = 3$  to  $n = 1$  ↓

☞ Electron transition: higher to lower level

☞ Emission

## EXAMPLE 5

Calculate the wavelength (in nm) of a photon emitted by a hydrogen atom when its electron drops from the  $n = 5$  state to the  $n = 3$  state.





$$\Delta E = R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad n_i = \text{initial}, n_f = \text{final}$$

$$= 2.18 \times 10^{-18} \text{ J} \times (1/25 - 1/9)$$

$$= -1.55 \times 10^{-19} \text{ J} \quad (\text{energy emitted})$$

$$\Delta E = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E}$$

$$= \frac{6.6256 \times 10^{-34} \text{ (Js)} \times 3.00 \times 10^8 \text{ (m/s)}}{1.55 \times 10^{-19} \text{ J}}$$

$$= 1.282 \times 10^{-6} \text{ m} = 1282 \text{ nm}$$

# RYDBERG EQUATION

- Used to calculate the **wavelength** of transition of electron between **two energy levels** :

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2$$

$\lambda$ : wavelength of a spectral line

$n_1, n_2$ : 1, 2, 3 ..... $\infty$

$R_H$ : Rydberg constant =  **$1.097 \times 10^7 \text{ m}^{-1}$**

**$\lambda > 0$ ,  $n_1 < n_2$**

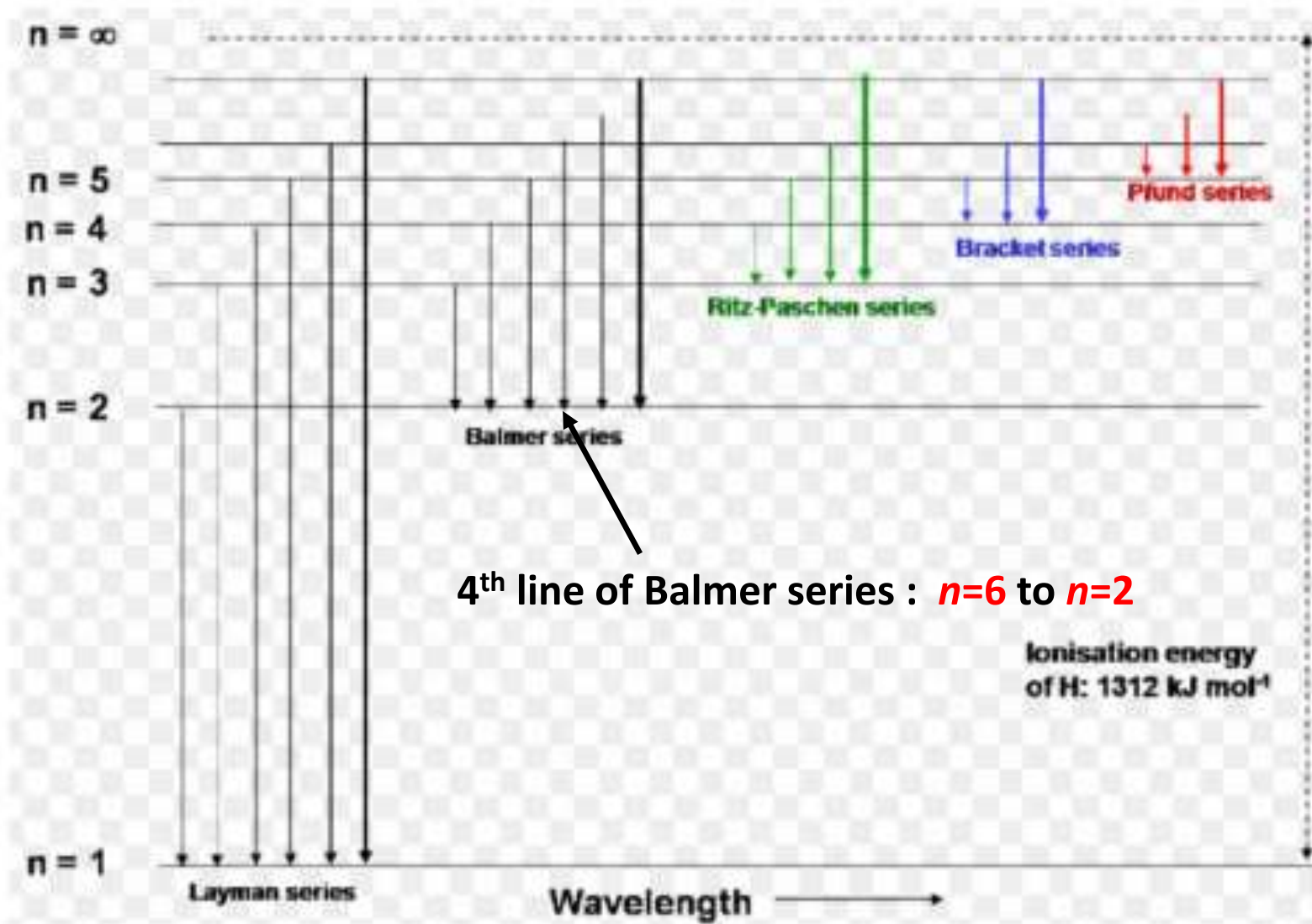
## EXAMPLE 6

Use the Rydberg equation to calculate:

- i. wavelength (in nm)
- ii. frequency
- iii. energy

of the **fourth line** in the **Balmer series** of hydrogen spectrum .







4<sup>th</sup> line of Balmer series :  $n=6$  to  $n=2$

By using Rydberg equation:

i)

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2$$

$$= 1.097 \times 10^7 \text{ m}^{-1} \left( \frac{1}{2^2} - \frac{1}{6^2} \right)$$

$$= 2.437 \times 10^6 \text{ m}^{-1}$$

$$\lambda = 4.102 \times 10^{-7} \text{ m} = 410.2 \text{ nm}$$

ii)

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

$$= \frac{3.00 \times 10^8 \text{ (m/s)}}{4.102 \times 10^{-7} \text{ m}}$$

$$= 7.314 \times 10^{14} \text{ s}^{-1}$$

iii)

$$\Delta E = h\nu$$

$$= 6.6256 \times 10^{-34} \text{ J}\cdot\cancel{\text{s}} \times 7.314 \times 10^{14} \cancel{\text{s}^{-1}}$$

$$= 4.845 \times 10^{-19} \text{ J}$$

## EXAMPLE 7

**An electron in the  $n = 5$  level of an H atom emits a photon of wavelength 1281 nm. To which energy level does the electron move?**

*ANS:  $n = 3$*

Electron transition:  $n_1 = 5$   $n_2 = ?$



By using Rydberg equation:

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2$$

$$\frac{1}{1281 \times 10^{-9} \text{ m}} = 1.097 \times 10^7 \text{ m}^{-1} \left( \frac{1}{n_1^2} - \frac{1}{5^2} \right)$$

$$7.8064 \times 10^5 = 1.097 \times 10^7 \text{ m}^{-1} \left( \frac{1}{n_1^2} - \frac{1}{5^2} \right)$$

$$\frac{1}{n_1^2} = 0.11116$$

$$n_1^2 = 8.996$$

$$n_1 = 3$$

# DIFFERENT VALUE OF $R_H$ AND USAGE

- Used to calculate **wavelength**

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2$$

$R_H$ : Rydberg constant =  $1.097 \times 10^7 \text{ m}^{-1}$

- Used to calculate **energy**

$$\Delta E = R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad n_i = \text{initial}, n_f = \text{final}$$

$R_H$ : Rydberg constant =  $2.18 \times 10^{-18} \text{ J}$

# IONIZATION ENERGY OF H ATOM

- Ionization energy (IE) : minimum energy (in kJ/mol) required to remove an electron from a gaseous atom or ion in its ground state.



- H atom is ionised when an electron is removed from :

$$n_1 = 1 \quad \text{to} \quad n_2 = \infty$$

$$\begin{aligned} \Delta E &= R_H \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\ &= 2.18 \times 10^{-18} \text{ J} \times \left( \frac{1}{1^2} - \frac{1}{\infty^2} \right) \\ &= 2.18 \times 10^{-18} \text{ J} \end{aligned}$$

# IONIZATION ENERGY OF H ATOM

For removal of 1 mol electrons from 1 mol H atom:

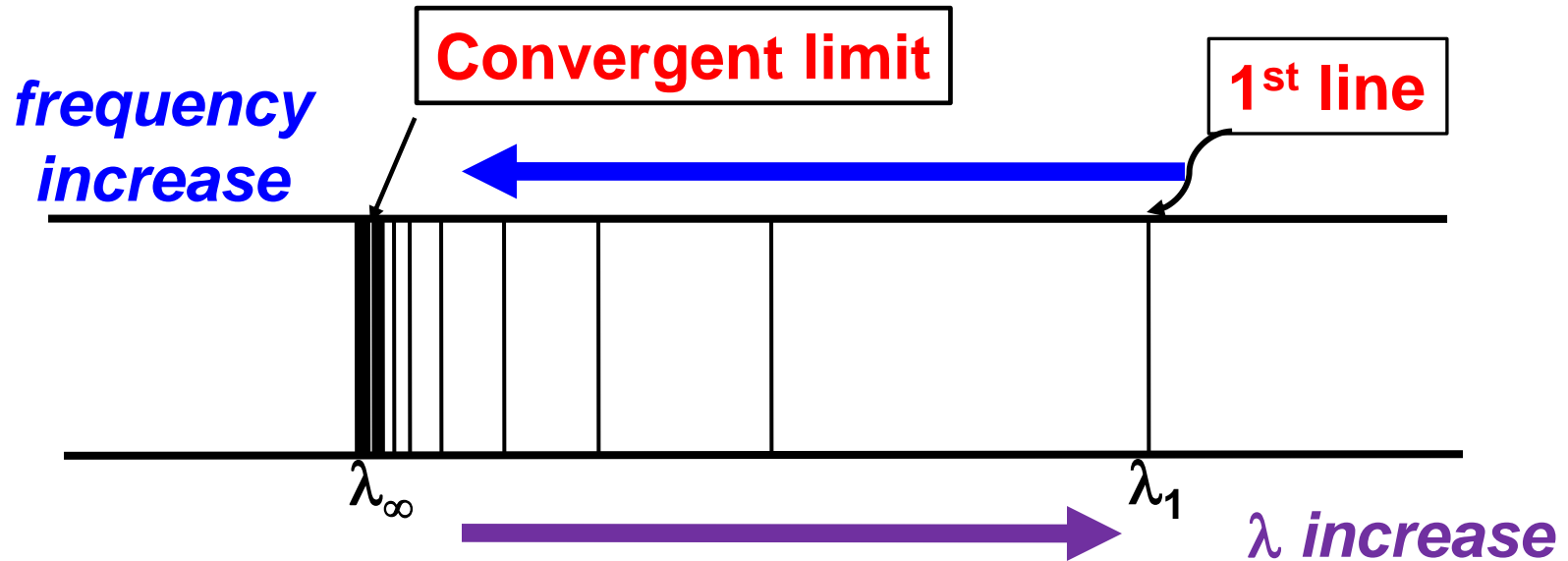
$$\Delta E = \frac{2.18 \times 10^{-18} \text{ J}}{1 \text{ atom H}} \times \frac{6.02 \times 10^{23} \text{ atoms H}}{1 \text{ mol}}$$

$$= 1.3124 \times 10^6 \text{ J/mol}$$

$$= 1312.4 \text{ kJ/mol}$$



## FINDING IONISATION ENERGY EXPERIMENTALLY:



- 👉 Ionisation energy is determined by detecting the **wavelength** of the convergence point.
- 👉 Eventually the line become so close to each other that merge at a point (**convergent limit/continuum limit**) form continuous band.
- 👉 the **nucleus** can **no longer** hold the electron.

## EXAMPLE 8

**Calculate the:**

- i) Wavelength**
- ii) Frequency**
- iii) Wave number**

**of the last line of hydrogen spectrum in Lyman series**

**NOTE:** Wave number =  $(1 / \text{wavelength})$  or  $1 / \lambda$



For Lyman series:  $n_1 = 1$  &  $n_2 = \infty$

$$\begin{aligned} \text{i)} \quad \frac{1}{\lambda} &= R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2 \\ &= 1.097 \times 10^7 \text{ m}^{-1} \times \left( \frac{1}{1^2} - \frac{1}{\infty^2} \right) \end{aligned}$$

$$\lambda = 9.116 \times 10^{-8} \text{ m}$$

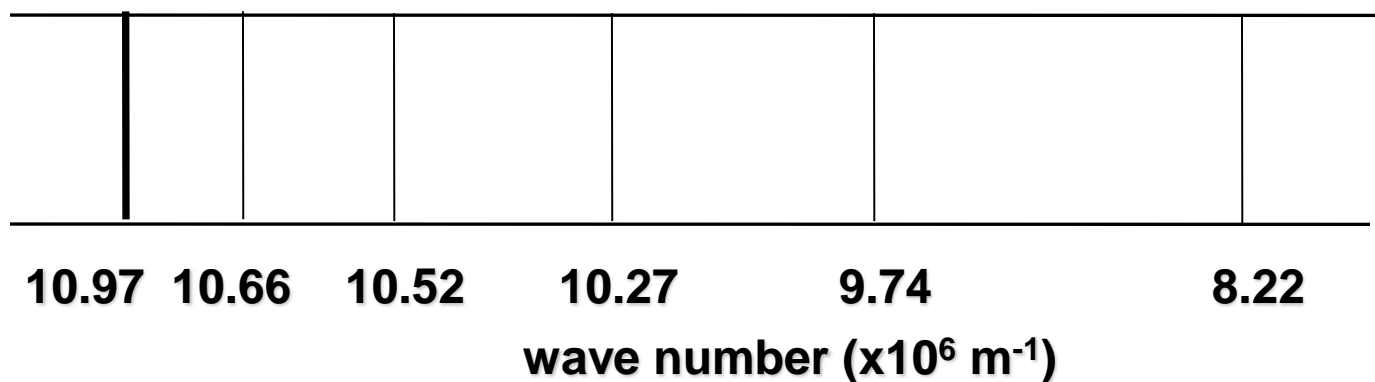
$$\begin{aligned} \text{ii)} \quad v &= \frac{c}{\lambda} \\ &= \frac{3.00 \times 10^8 \text{ (m/s)}}{9.116 \times 10^{-8} \text{ m}} \\ &= 3.291 \times 10^{15} \text{ s}^{-1} \end{aligned}$$

iii) Wave number ,  $\frac{1}{\lambda}$

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 < n_2$$
$$= 1.097 \times 10^7 \text{ m}^{-1} \times \left( \frac{1}{1^2} - \frac{1}{\infty^2} \right)$$

$$= 1.097 \times 10^7 \text{ m}^{-1}$$

## EXAMPLE 9



**The Lyman series of the spectrum of hydrogen is shown above. Calculate the ionisation energy of hydrogen from the spectrum.**

## EXAMPLE 9



$$\begin{aligned}\Delta E &= h \times \frac{c}{\lambda} \\ &= 6.6256 \times 10^{-34} \text{ (J}\cdot\text{s)} \times 3.00 \times 10^8 \text{ (m/s)} \times 10.97 \times 10^6 \text{ m}^{-1} \\ &= 218.06 \times 10^{-20} \text{ J} \\ &= 2.18 \times 10^{-18} \text{ J}\end{aligned}$$

For 1 mol of electrons:

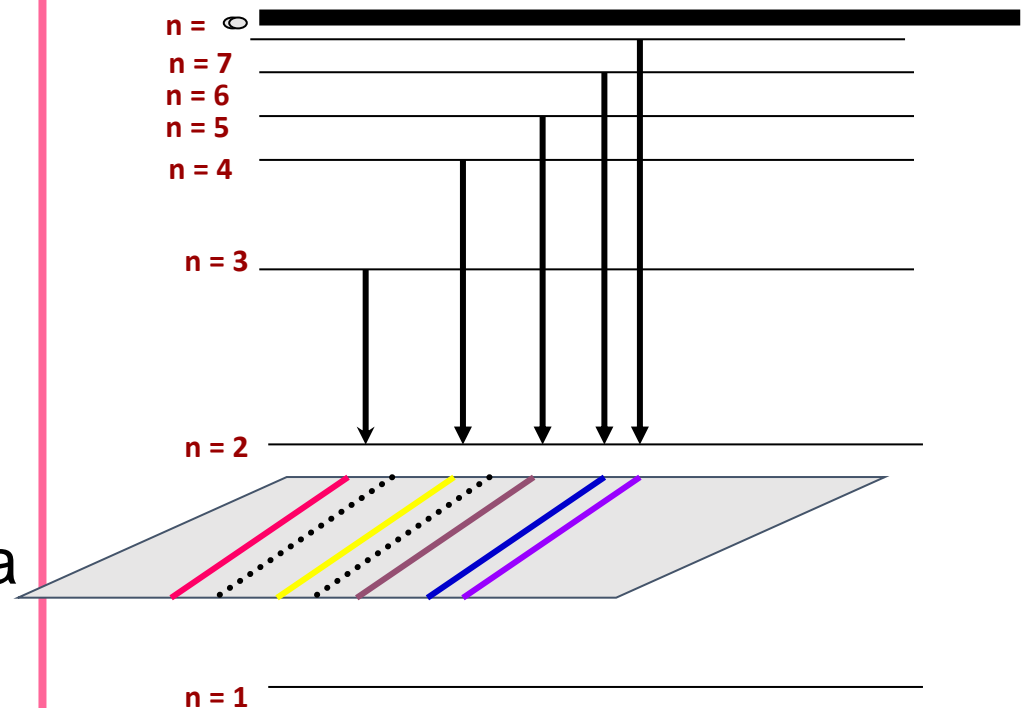
**Ionisation energy**

$$\begin{aligned}&= \frac{2.18 \times 10^{-18} \text{ J}}{1 \text{ atom H}} \times \frac{6.02 \times 10^{23} \text{ atom H}}{1 \text{ mol}} \\ &= 1.312 \times 10^6 \text{ J mol}^{-1} \\ &= 1312 \text{ kJ mol}^{-1}\end{aligned}$$

# Limitation of Bohr's atomic model

- ❑ Unable to explain the line spectrum of atoms or ions containing more than one electron (such as helium).
- ❑ Electron is restricted to move in a certain distance around the nucleus of an atom.
- ❑ Unable to explain the extra lines formed.
- ❑ Unable to explain the dual nature of electrons.

**Why got extra lines....?**



**BALMER SERIES**

# de Broglie's Postulates

- ❖ Tiny particles like electrons can also have wave properties
- ❖ Electrons should diffuse like wave into dimensionless space.
- ❖ Electrons **should NOT** be confined to a particular energy level.

Wave  
property

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

Particle  
property

Where:

$h$  = Planck constant (J.s)

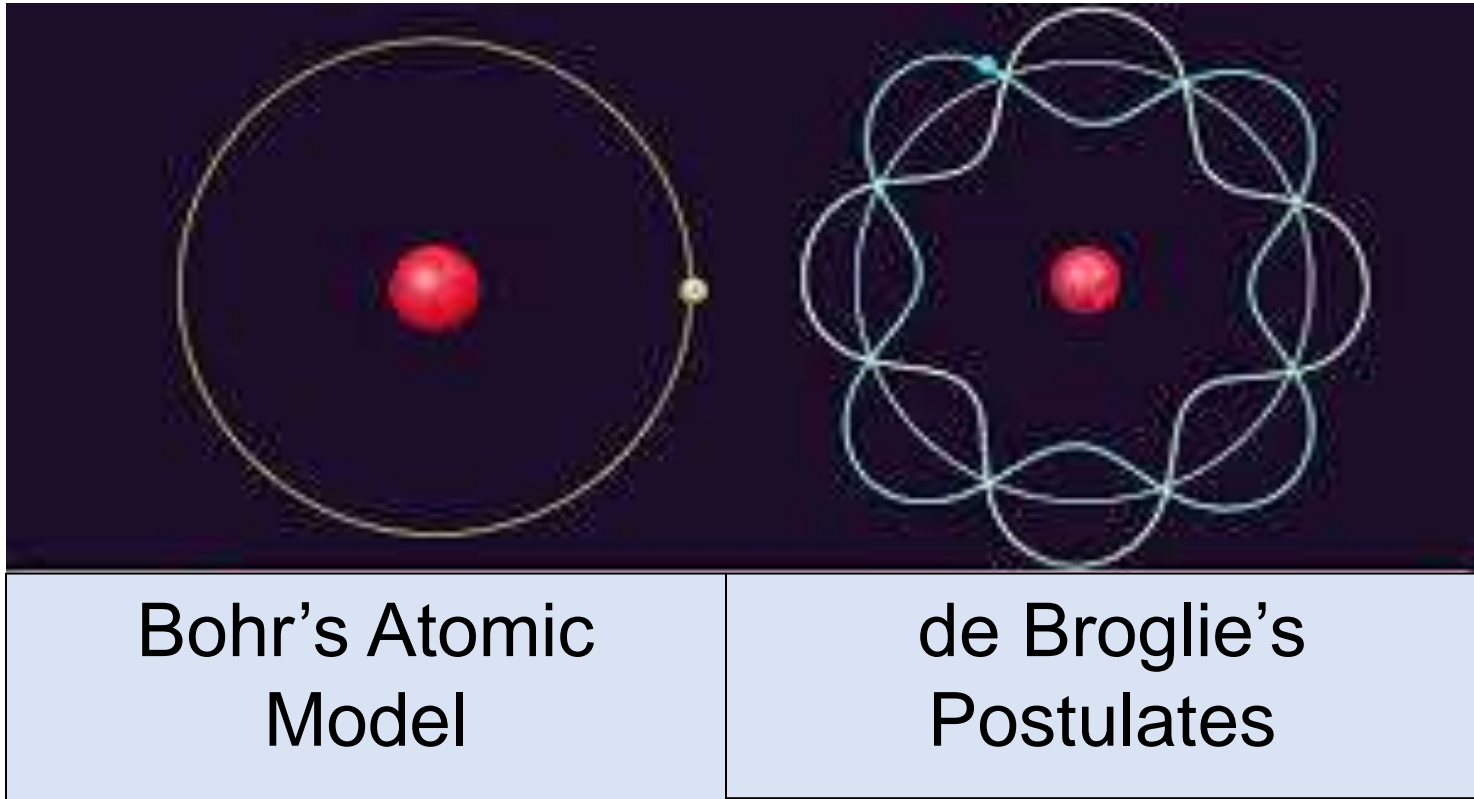
$u$  = velocity (m/s)

$m$  = particle mass (kg)

$\lambda$  = wavelength



# de Broglie's Postulates



# Heisenberg's Uncertainty Principle

- ❖ It is impossible to know simultaneously both the **momentum,  $p$**  and the **position,  $x$**  of a moving particle with certainty.
- ❖ An electron should not be confined in a particular orbit because its **exact position** and **velocity** cannot be determined
- ❖ We can only determine the **probability** of finding an electron.

Where:

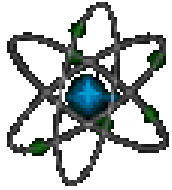
$\Delta x$  = uncertainty in measuring the position

$\Delta p$  = uncertainty in measuring the momentum

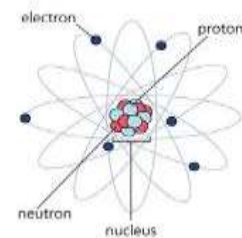
$h$  = Planck's constant

$\pi$  = pi

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$



## 2.2 QUANTUM MECHANICAL MODEL

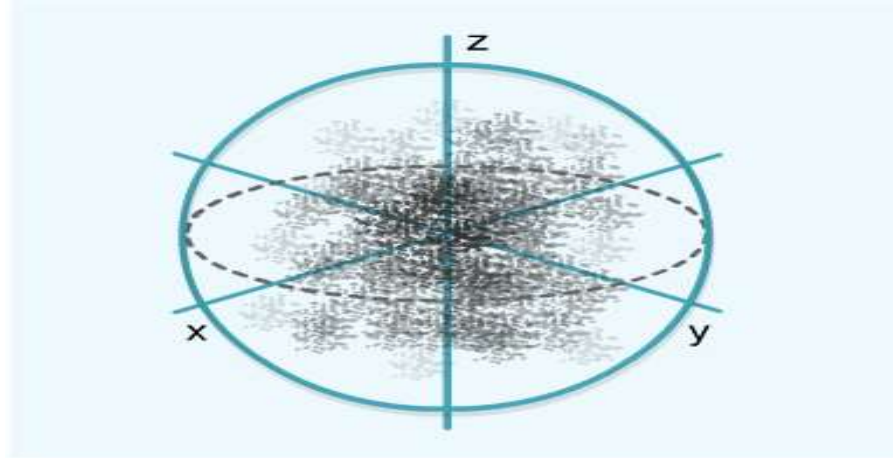


# Learning Outcomes:

## 2.2 Quantum Mechanics model.

- a) Define the term orbital.
- b) Explain all four quantum numbers of an electron in an orbital:
  - i. principal quantum number,  $n$
  - ii. angular momentum quantum number,  $\ell$
  - iii. magnetic quantum number,  $m$
  - iv. electron spin quantum number,  $s$
- c) Sketch the 3-D shapes of  $s$ ,  $p$  and  $d$  orbitals.

# ATOMIC ORBITAL



An orbital is a three-dimensional **region** in space **around the nucleus** where there is a **high probability** of finding an electron.

# QUANTUM NUMBER

■ For H atom, an atomic orbital is specified by 4 quantum numbers :

1

Principal quantum number ( $n$ )

■ indicates the *energy level* of the electron

2

Angular momentum quantum number ( $\ell$ )

■ indicates the *shape of the orbital*

3

Magnetic quantum number ( $m$ )

■ describes the *orientation* of the orbital in space



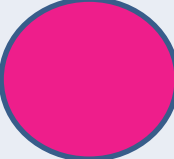
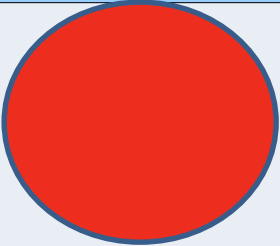

4

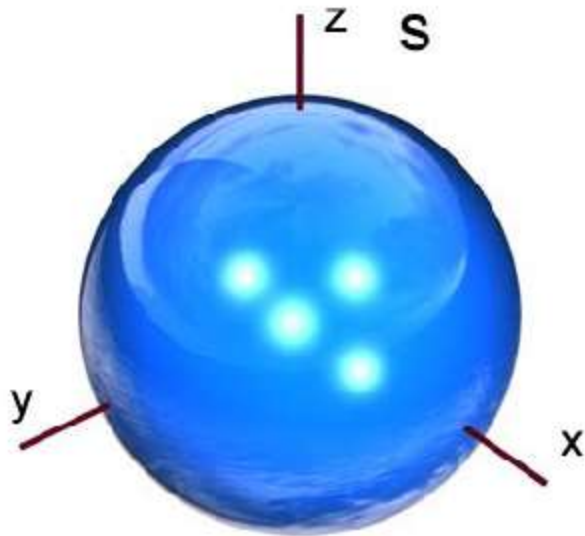
Electron spin quantum number ( $s$ )

■ represents the *spin direction* of electron on its own axis

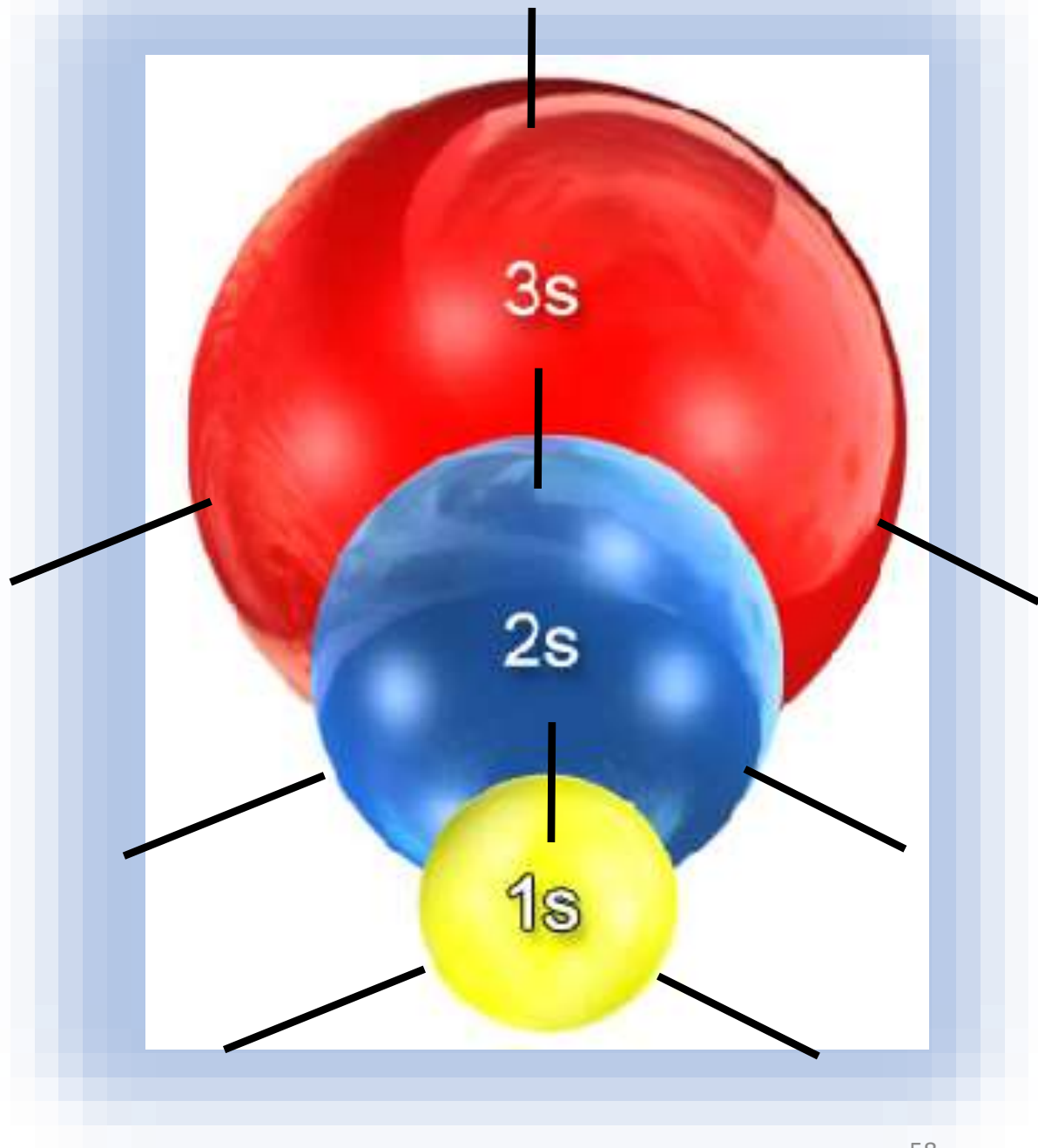
# PRINCIPAL QUANTUM NUMBER ( $n$ )

- The **value** of  $n$  determines the **size** and **energy** of an atomic orbital.
- The principal quantum number may have only **positive integers**:  $n = 1, 2, 3, \dots, \infty$

$n$	1	2	3	4
Orbital size				
Energy	Increase 			



Orbital size:  
 $3s > 2s > 1s$





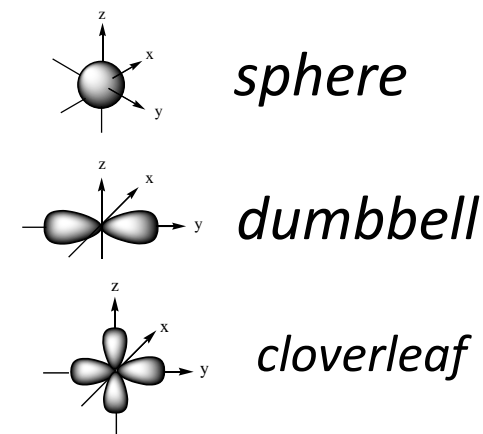
# ANGULAR MOMENTUM QUANTUM NUMBER ( $\ell$ )

- Also called **azimuthal** / **subsidiary** / **orbital quantum number**
- $\ell$  = An integer from **0** to  **$(n - 1)$**  @  $\ell = (n - 1)$
- Indicates **shape** and **type** of orbital
- $n$  determine  $\ell$

$n$	$\ell$	Subshell
<b>1</b>	<b>0</b>	1s
<b>2</b>	<b>0</b>	2s
	<b>1</b>	2p
<b>3</b>	<b>0</b>	3s
	<b>1</b>	3p
	<b>2</b>	3d

Note :

$\ell$	orbital
<b>0</b>	<b>s</b>
<b>1</b>	<b>p</b>
<b>2</b>	<b>d</b>
<b>3</b>	<b>f</b>



# MAGNETIC QUANTUM NUMBER ( $m$ )

- $m$  = an integer from  $-\ell$  through 0 to  $+\ell$  @  $m=(-\ell..0..+\ell)$
- Indicates the **orientation** of the **orbital** in the **space around the nucleus**
- $m$  depends on the value of  $\ell$

## EXAMPLE:

$$\ell = 0$$

$$m = 0$$

1 possible orbitals  
( s subshell)

$$\ell = 1$$

$$m = -1, 0, +1$$

3 possible orbitals  
( p subshell)

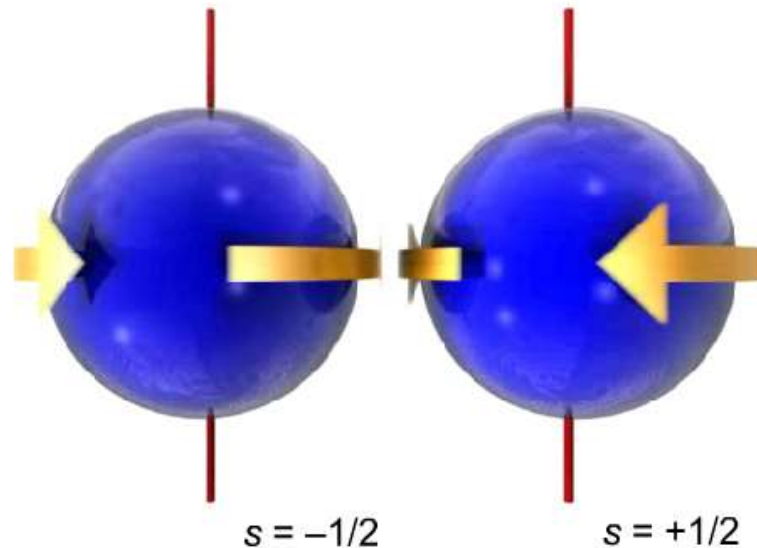
$$\ell = 2$$

$$m = -2, -1, 0, +1, +2$$

5 possible orbitals  
( d subshell)

# ELECTRON-SPIN QUANTUM NUMBER ( $s$ )

- determines the direction of spinning motions of an electron
- Two possible motions of an electron  
☞ clockwise and anti-clockwise
- value of  $s$ :  $+\frac{1}{2}$  and  $-\frac{1}{2}$



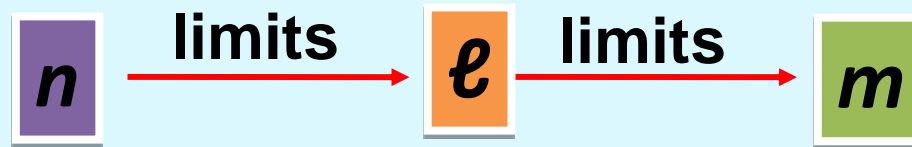
■ Each **allowed combination** of  $n$ ,  $\ell$  and  $m$  values specifies **one atomic orbital**

☞ size (energy), **shape** and spatial **orientation**

n	$\ell$	m	Orbitals (name)	Number of orbitals	Number of e <sup>-</sup>
1	0	0	1s	1	2
2	0	0	2s	1	2
	1	-1, 0, +1	2p	3	6
3	0	0	3s	1	2
	1	-1, 0, +1	3p	3	6
	2	-2, -1, 0, +1, +2	3d	5	10

## POINT TO REMEMBER

- Hierarchical relationship:



### EXAMPLE:

$n = 2$       possible  $\ell$  values = 0 , 1

$\ell = 1$       possible  $m$  values = - 1 , 0 , +1

$\ell = 0$       possible  $m$  values = 0

- max no. of  $e^-$  =  $2n^2$

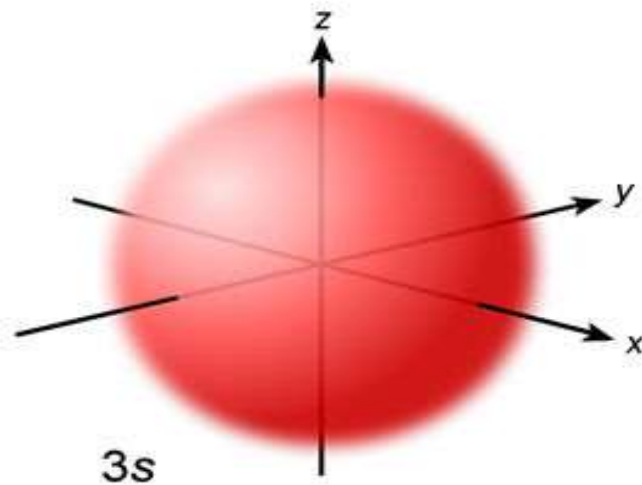
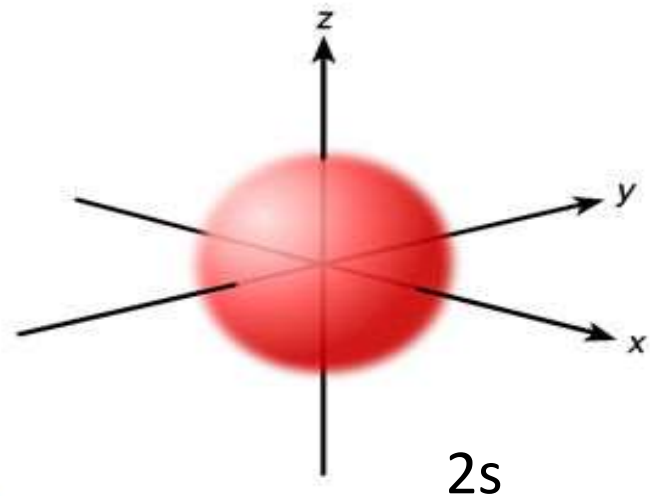
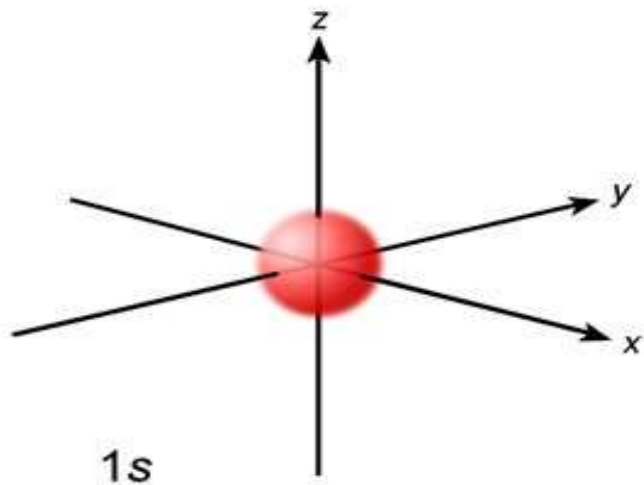
# SHAPE OF *ATOMIC* ORBITAL

## s orbital

- The s orbital is represented by  $l = 0$
- It has **spherical shape** with the nucleus at the centre.
- The  $l = 0$  , there is only one value of  $m = 0$ , which refer to **one s orbital**
- The size of s orbital becomes **larger** as the value of **n increases**

# SHAPE OF $s$ ORBITAL

- The size of  $s$  orbital with different values of  $n$



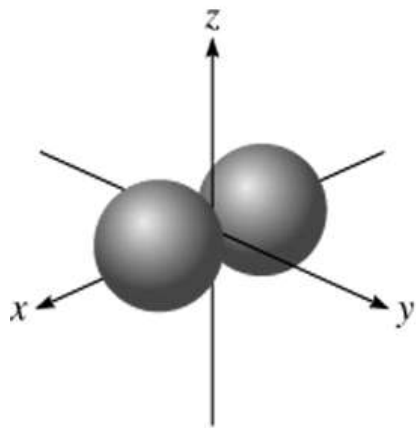
# SHAPE OF *ATOMIC* ORBITAL

## p orbital

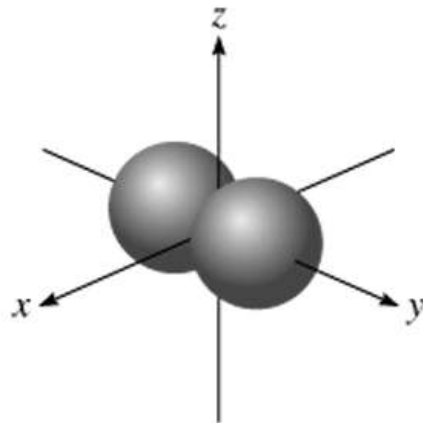
- The p orbitals are represented by  $l = 1$
- Each p orbitals has **dumbbell shaped** and separated by a node at the nucleus
- The  $l = 1$  , there are **three possible values** of  $m = -1, 0, +1$ , which refer to three p orbitals, ( $p_x, p_y, p_z$ )
- As **n increases**, the p orbitals get **larger**



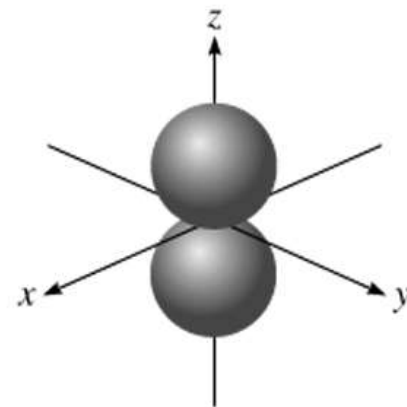
# SHAPE OF $p$ ORBITAL



$P_x$



$P_y$



$P_z$

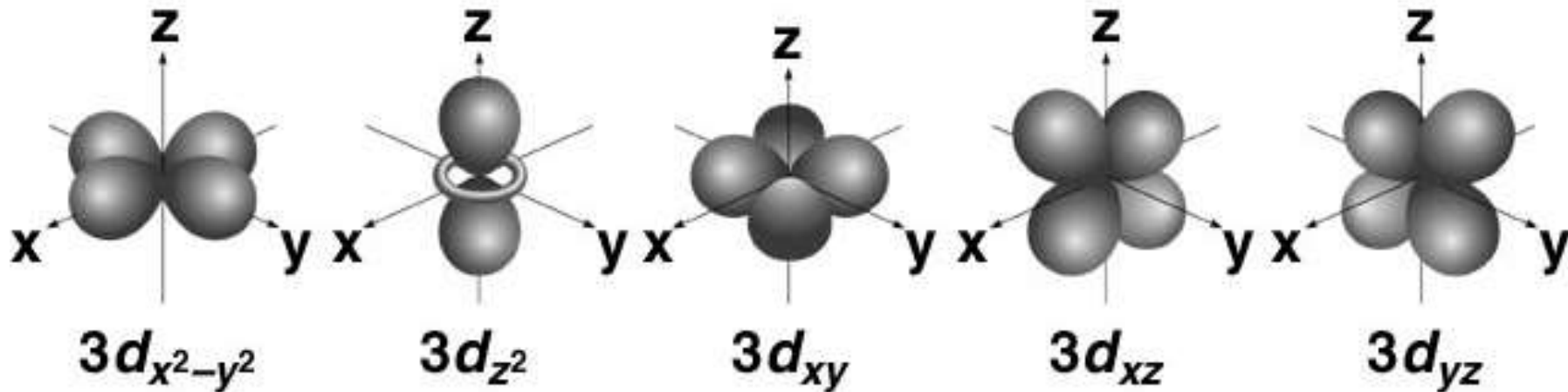
# SHAPE OF *ATOMIC* ORBITAL

## d orbital

- The d orbitals are represented by  $l = 2$
- All the d orbitals do **not look alike**.
- There are five possible m values: **-2, -1, 0, +1, +2**, which correspond to **five d orbitals** with five different orientations:

$$d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$$

# SHAPE OF $d$ ORBITAL



## EXAMPLE 10

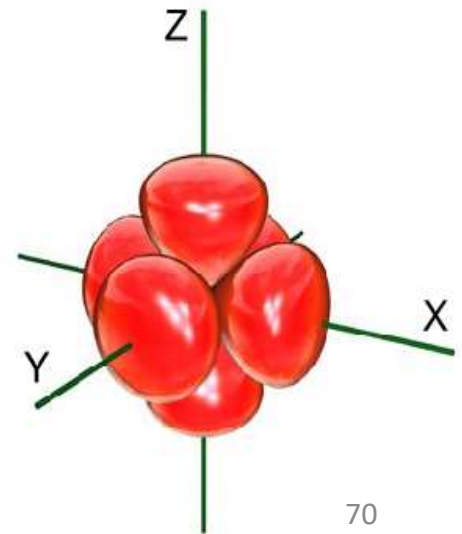
Specify the  $\ell$  and  $m$  values for  $n = 4$ .



When,  $n = 4$

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

$\ell$	$m$
0	0
1	-1, 0, +1
2	-2, -1, 0, +1, +2
3	-3, -2, -1, 0, +1, +2, +3



## EXAMPLE 11



Give all possible  $m$  values for orbitals that have each of the following:

a)  $\ell = 2$

When  $\ell = 2$ ,

Possible values of  $m = -2, -1, 0, +1, +2$

b)  $n = 4, \ell = 3$

When  $n = 4, \ell = 3$

$\ell = 3$

Possible values of  $m = -3, -2, -1, 0, +1, +2, +3$

## EXAMPLE 12

**Give the name, magnetic quantum numbers, and number of orbitals for each subshell with the following quantum numbers:**

**a)  $n = 3$  ,  $\ell = 2$**

**b)  $n = 2$  ,  $\ell = 0$**

**c)  $n = 5$  ,  $\ell = 1$**

**d)  $n = 4$  ,  $\ell = 3$**

## EXAMPLE 12



	$n$	$\ell$	Name of orbital	Possible $m$ values	Number of orbitals
a)	3	2	$3d$	$-2, -1, 0, +1, +2$	5
b)	2	0	$2s$	0	1
c)	5	1	$5p$	$-1, 0, +1$	3
d)	4	3	$4f$	$-3, -2, -1, 0, +1, +2, +3$	7

## EXAMPLE 13



Are the following quantum number combinations allowed? If not, show two ways to correct them.

a)  $n = 1; \ell = 0; m = -1$

When  $n = 1; \ell = 0$

$$\ell = 0; m = 0 \quad m \neq -1$$

So, the combination is not allowed.

Correction:

$$n = 1; \ell = 0; m = 0 \quad \text{or} \quad n = 2; \ell = 1; m = -1$$



## EXAMPLE 13



b)  $n = 4; \ell = 3; m = -1$

When  $n = 4; \ell = 0, 1, 2, 3$

$$\ell = 3; m = -3, -2, -1, 0, +1, +2, +3$$

So, the combination is **allowed**.

## EXAMPLE 13



c)  $n = 5; \ell = 2; m = +3$

When  $n = 5; \ell = 0, 1, 2, 3, 4$

$$\ell = 2; m = -2, -1, 0, +1, +2 \quad m \neq +3$$

Combination is not allowed.

Correction:

$$n = 5; \ell = 2; m = +2$$

or

$$n = 5; \ell = 3; m = +3$$

## EXAMPLE 14



For the following subshells give the values of the quantum numbers ( $n$ ,  $\ell$ ,  $m$ ) and the number of orbitals in each subshell:

a)  $3p$

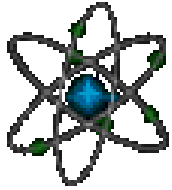
$n = 3$ ,  $\ell = 1$ ,  $m = -1, 0, +1$  (3 orbitals)

b)  $5d$

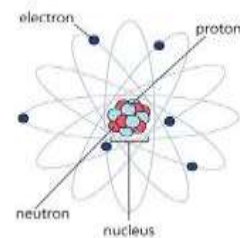
$n = 5$ ,  $\ell = 2$ ,  $m = -2, -1, 0, +1, +2$  (5 orbitals)

c)  $4f$

$n = 4$ ,  $\ell = 3$ ,  $m = -3, -2, -1, 0, +1, +2, +3$  (7 orbitals)



## 2.3 ELECTRONIC CONFIGURATION



# Learning Outcomes:

## 2.3 Electronic Configuration.

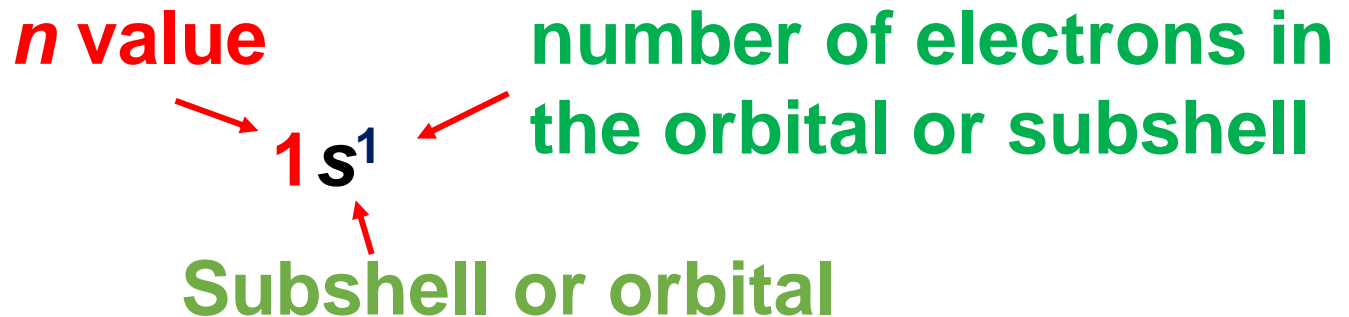
- a) Explain Aufbau principle, Hund's rule and Pauli exclusion principle.
- b) Predict the electronic configuration of atoms and monoatomic ions using *spdf* notation and orbital diagram.
- c) Justify the anomalous electronic configurations of copper and chromium.

# ELECTRONIC CONFIGURATION

- Shows how the **electrons** are **distributed** among the **various atomic orbitals**

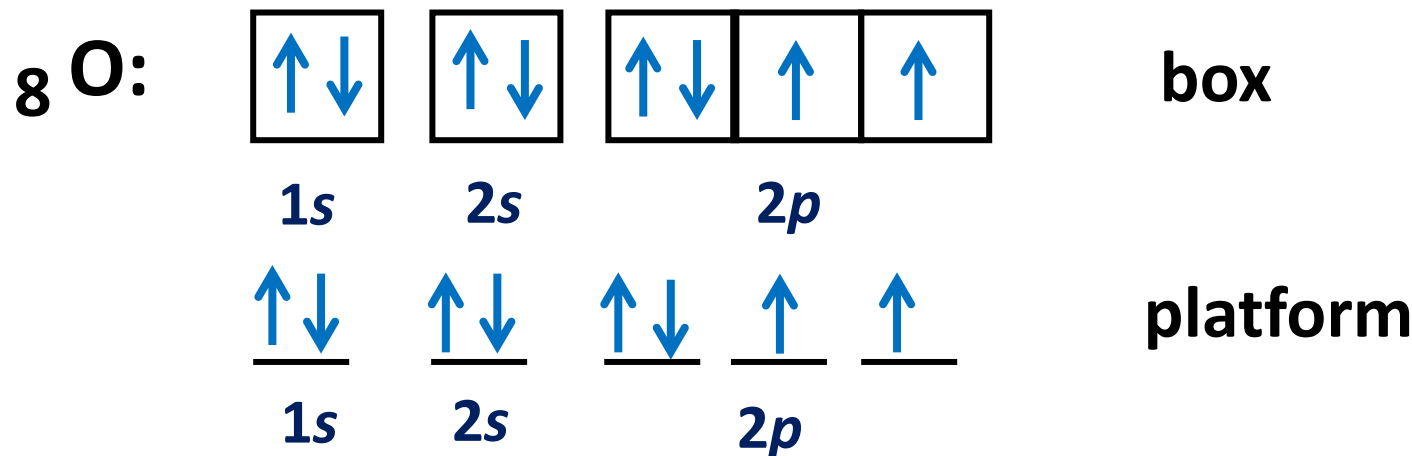
## EXAMPLE:

H atom (ground state)

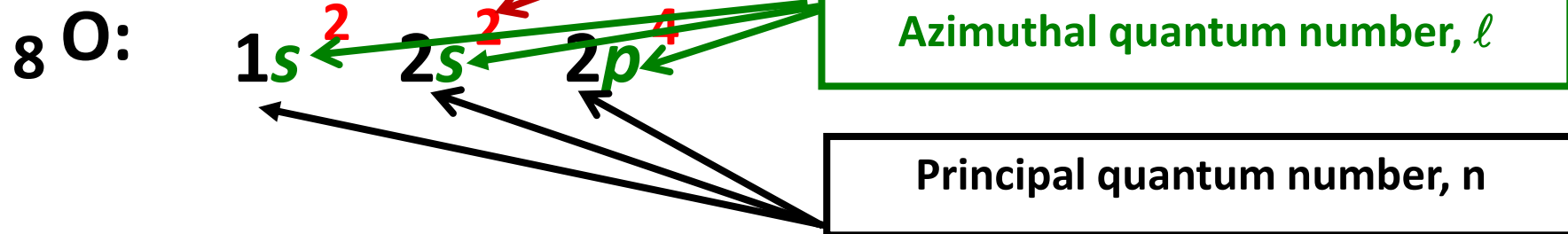


# Representing Electronic Configuration

## Method 1: Orbital diagram



## Method 2: *spdf* notation



# **Rules Used to Fill Electrons Into Atomic Orbitals**

**Aufbau Principle**

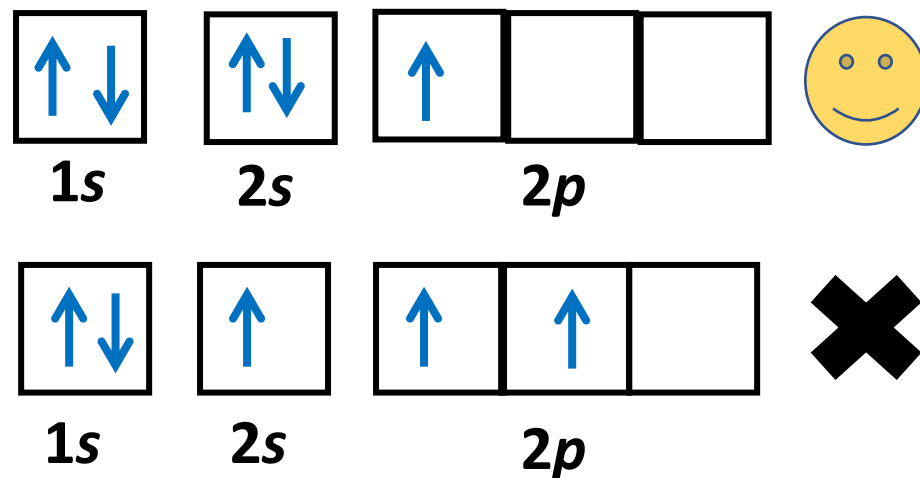
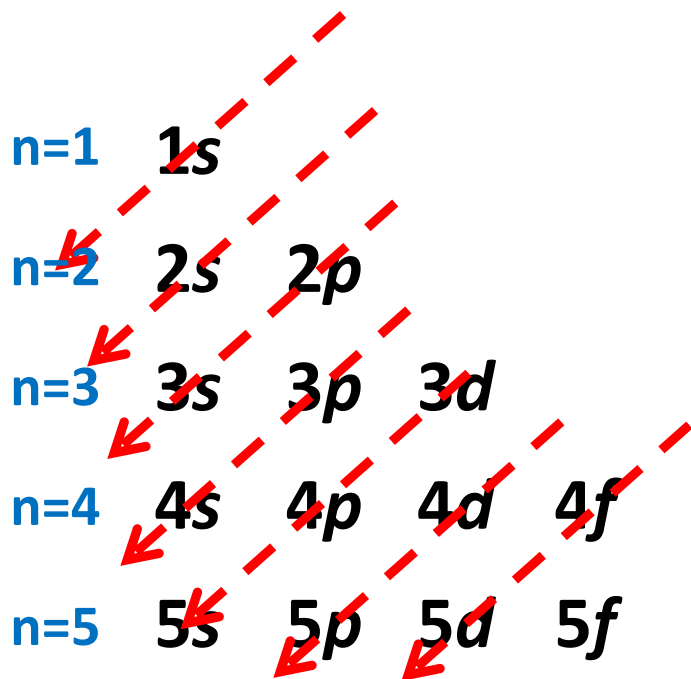
**Hund's Principle**

**Pauli Exclusion Principle**



# AUFBAU PRINCIPLE

Electrons fill the **lowest energy orbitals first** and other orbitals in **order of increasing energy**.



The order of filling energy orbitals with electrons:

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s$$

# KEEP IN MIND



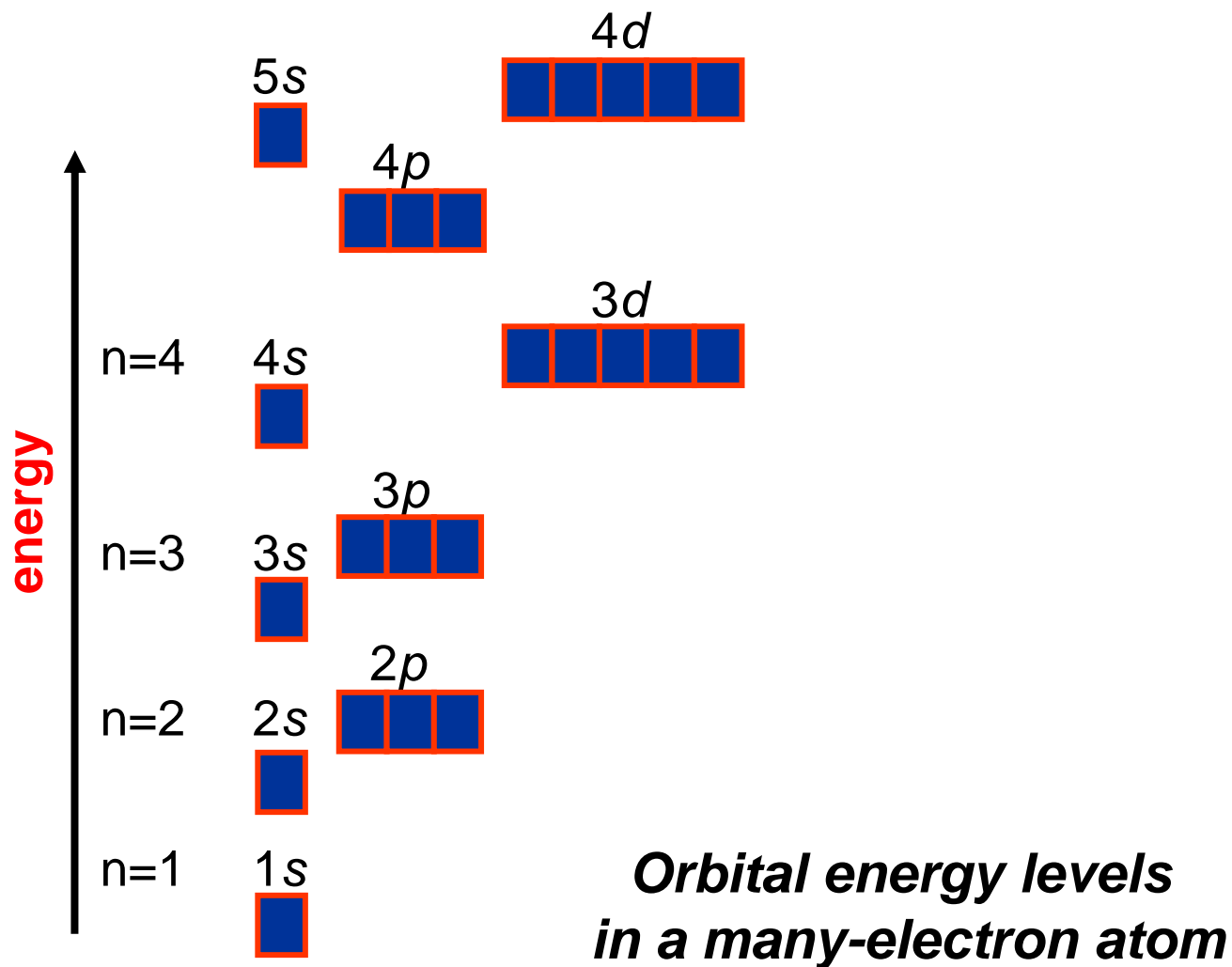
**Degenerate orbitals** are **orbitals** with the same energy.

## EXAMPLE:

$$2p_x = 2p_y = 2p_z$$

$$3d_{xy} = 3d_{yz} = 3d_{xz} = 3d_{x^2 - y^2} = 3d_z^2$$

# Relative Energy Level of Atomic Orbitals



## EXAMPLE 15

Which of the following pairs is lower in energy for the case of many-electron atoms:

a)  $2s$  ,  $2p$        $2s < 2p$

b)  $3p$  ,  $3d$        $3p < 3d$

c)  $3s$  ,  $4s$        $3s < 4s$

d)  $4d$  ,  $5f$        $4d < 5f$

e)  $3d$  ,  $4s$        $4s < 3d$

# PAULI EXCLUSION PRINCIPLE

- No two electrons in the same atom have the same four quantum numbers



In other words,

- Each electron must have a different set of quantum numbers

## EXAMPLE:

He atom  
 $1s^2$

1<sup>st</sup> electron

$(1, 0, 0, +\frac{1}{2})$

$(1, 0, 0, -\frac{1}{2})$

$(1, 0, 0, +\frac{1}{2})$

2<sup>nd</sup> electron

$(1, 0, 0, +\frac{1}{2})$

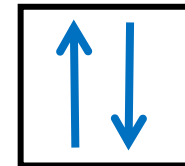
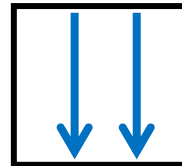
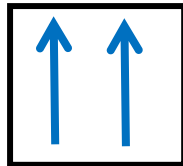
$(1, 0, 0, -\frac{1}{2})$

$(1, 0, 0, -\frac{1}{2})$

WRONG  
WAY

WRONG  
WAY

☒ correct

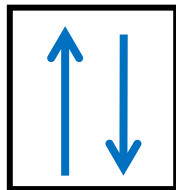


# HUND'S RULE

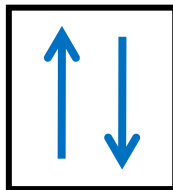
Most stable arrangement of electrons in orbital of a subshell is **the one with the greatest number of parallel spin**

Thus electrons fill each and all degenerate orbital singly before they pair up.

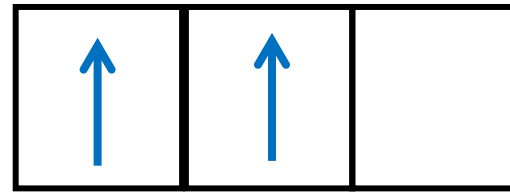
C ( $Z = 6$ )



1s



2s



2p

number of parallel  
spin = **2**

# HOW TO WRITE ELECTRONIC CONFIGURATION OF AN ION?



**Write electronic configuration for the respective neutral atom**



**Cation: remove first electron from the outermost shell**

**Anion: add electron to the outermost shell**



## EXAMPLE 16

Write the electron configuration of K ( $Z = 19$ ) and Mg ( $Z = 12$ ).



K :  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

Mg:  $1s^2 2s^2 2p^6 3s^2$





## EXAMPLE 17

**Write the electron configuration of the following transition metal:**

- a)  $V^{5+}$  (V;  $Z = 23$ )**
- b)  $Ti^{4+}$  (Ti;  $Z = 22$ )**
- c)  $Sc^{3+}$  (Sc;  $Z = 21$ )**
- d)  $N^{3-}$  (N;  $Z = 7$ )**
- e)  $S^{2-}$  (S;  $Z = 16$ )**

## EXAMPLE 17



a)  $V^{5+}$

Electron configuration:

$V : 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$

or

$V : 1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$



$V^{5+}$  (18 electrons)

$V^{5+} : 1s^2 2s^2 2p^6 3s^2 3p^6$

## EXAMPLE 17



b)  $\text{Ti}^{4+}$  (Ti;  $Z = 22$ )

Ti (22 electrons)

Electron configuration:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$

or

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$



$\text{Ti}^{4+}$  (18 electrons)

$1s^2 2s^2 2p^6 3s^2 3p^6$

## EXAMPLE 17



c)  $\text{Sc}^{3+}$  (Sc;  $Z = 21$ )

Sc (21 electrons)

Electron configuration:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

or

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$



$\text{Sc}^{3+}$  (18 electrons)

$1s^2 2s^2 2p^6 3s^2 3p^6$

## EXAMPLE 17

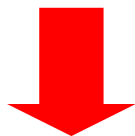


d)  $\text{N}^{3-}$  (N;  $Z = 7$ )

N (7 electrons)

Electronic configuration:

$1s^2 2s^2 2p^3$



$\text{N}^{3-}$  (10 electrons)

$1s^2 2s^2 2p^6$

## EXAMPLE 17



e)  $\text{S}^{2-}$  (S;  $Z = 16$ )

S (16 electrons)

Electronic configuration:

$1s^2 2s^2 2p^6 3s^2 3p^4$



$\text{S}^{2-}$  (18 electrons)

$1s^2 2s^2 2p^6 3s^2 3p^6$

# The Anomalous Electronic Configurations of Chromium, Cr and Copper, Cu

- ➡ **Cr** and **Cu** both have electron configurations which are **inconsistent with the Aufbau Principle**
- ➡ The anomalies are explained on the basis that a **fully filled** or **half-filled d orbital** is **more stable**.

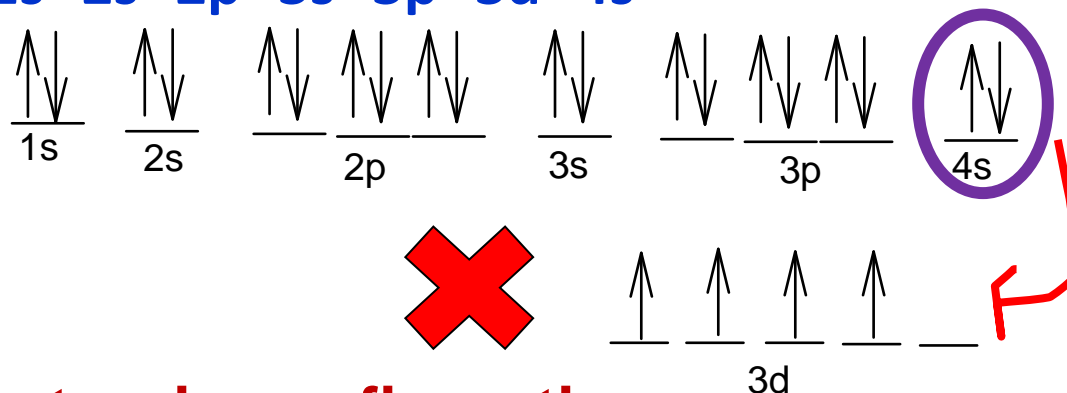
Element	Expected e <sup>-</sup> configuration	Observed/actual e <sup>-</sup> configuration
Cr (Z=24)	[Ar] <b>3d<sup>4</sup> 4s<sup>2</sup></b>	[Ar] <b>3d<sup>5</sup> 4s<sup>1</sup></b>
Cu (Z=29)	[Ar] <b>3d<sup>9</sup> 4s<sup>2</sup></b>	[Ar] <b>3d<sup>10</sup> 4s<sup>1</sup></b>

# Anomalous Cases

Chromium (Z=24)

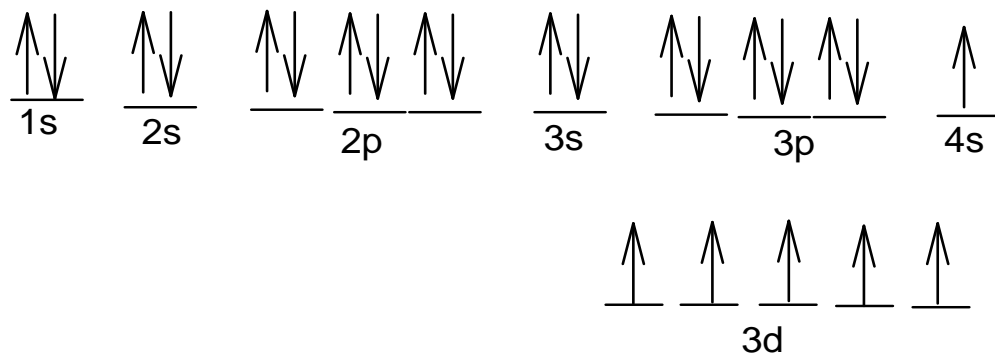
**Expected electronic configuration:**

${}_{24}\text{Cr} : 1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2$



**Actual electronic configuration:**

${}_{24}\text{Cr} : 1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$



**REASON:**

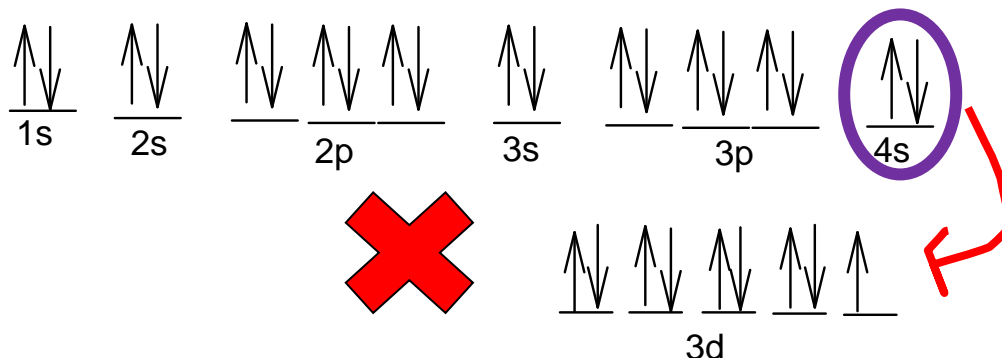
**Half-filled ( $3d^5$ ) orbitals exhibits greater stability**



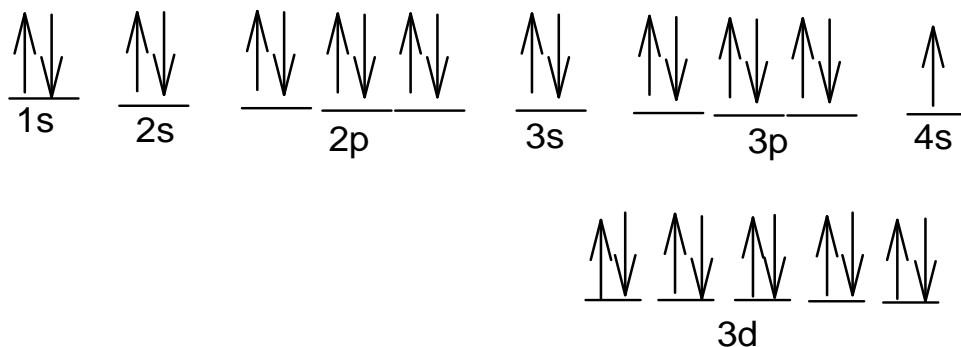
# Anomalous Cases

Copper (Z=29)

## Expected electronic configuration:



## Actual electronic configuration:



### REASON:

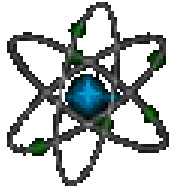
Fully filled ( $3d^{10}$ ) orbitals exhibits greater stability

# GLOSSARY

BIL	TERM	SYMBOL/ FORMULA	DEFINE
1.	Energy level	-	Energy associated with a specific orbit or state
2.	Ground state	-	The electrons have their lowest energy
3.	<i>Photon</i>	-	A packet of light energy equals to $h\nu$
4.	Continuous Spectrum	-	A spectrum that contains continuous bands of light with all wavelengths.
5.	Line Spectrum	-	A spectrum that contains a series of discrete lines separated by blank area and each line corresponds to specific wavelength.
6.	de Broglie's Postulates	-	Tiny particles like electrons can also have wave properties.
7.	Heisenberg's Uncertainty Principle	-	It is impossible to know simultaneously both the momentum, $p$ and the <i>position</i> , $x$ of a moving particle with certainty.
8.	Atomic Orbital	-	An orbital is a three-dimensional region in space around the nucleus where there is a high probability of finding an electron.

# GLOSSARY

BIL	TERM	SYMBOL/ FORMULA	DEFINE
9.	Principal quantum number ( $n$ )	$n = 1, 2, 3, \dots, \infty$	indicates the energy level of the electron
10.	Angular momentum quantum number ( $\ell$ )	0 to $(n - 1)$	indicates the shape of the orbital
11.	Magnetic quantum number ( $m$ )	$m = (-\ell..0..+\ell)$	describes the orientation of the orbital in space
12.	Electron spin quantum number ( $s$ )	$s: +\frac{1}{2}$ and $-\frac{1}{2}$	represents the spin direction of electron on its own axis.
13.	Electronic Configuration		Shows how the electrons are distributed among the various atomic orbitals.
14.	Aufbau Principle		Electrons fill the lowest energy orbitals first and other orbitals in order of increasing energy.
15.	Pauli Exclusion Principle		No two electrons in the same atom have the same four quantum numbers.  or Each electron must have a different set of quantum numbers
16.	Hund's Rule		Most stable arrangement of electrons in orbital of a subshell is the one with the greatest number of parallel spin



# THE END

