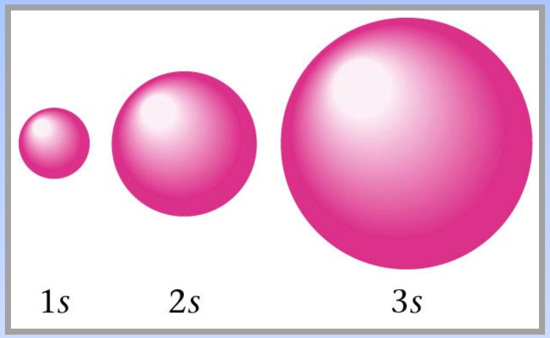
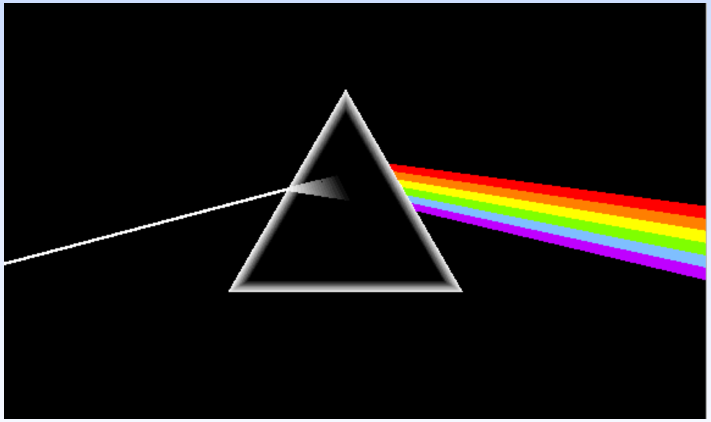
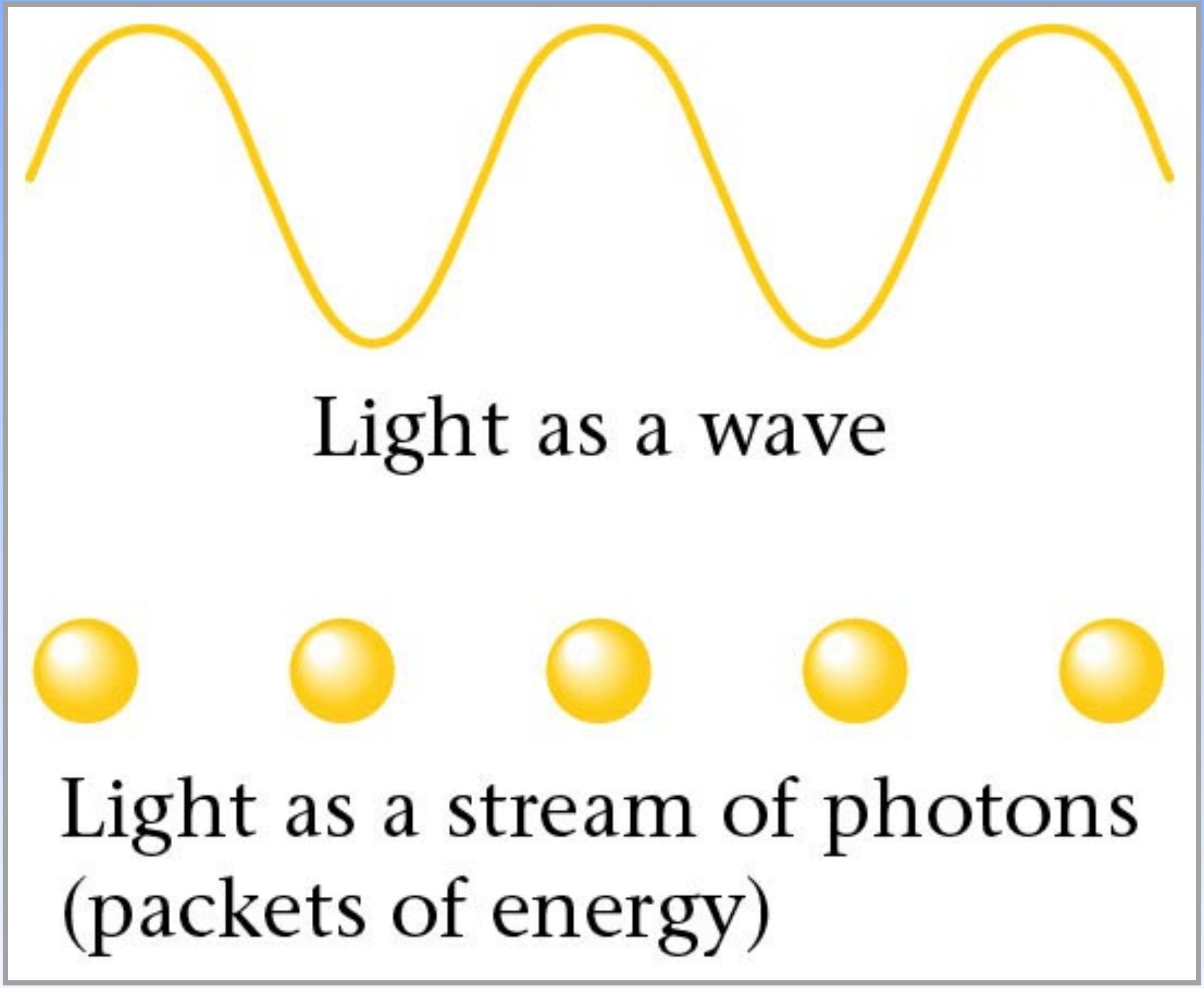
Modern Atomic Theory
(a.k.a. the electron!)





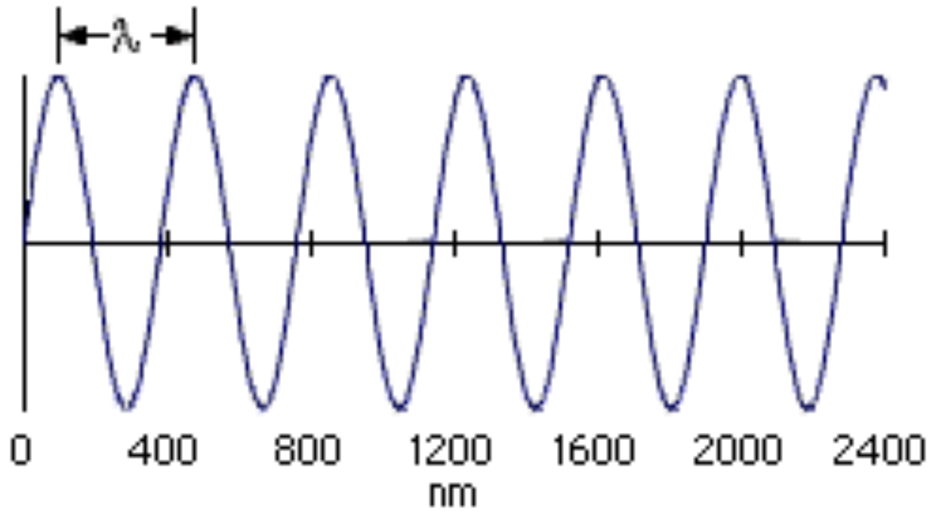
ELECTROMAGNETIC RADIATION

Electromagnetic radiation.

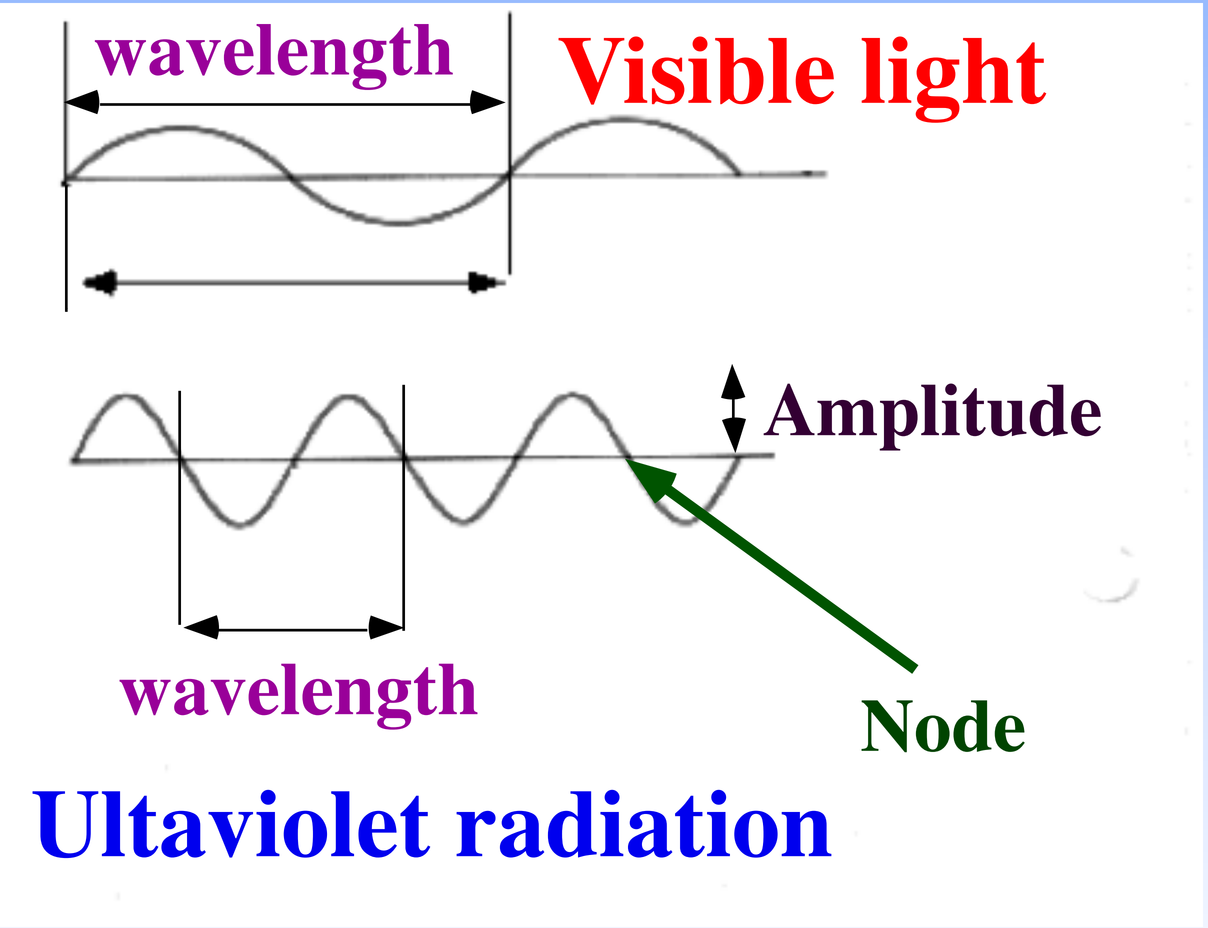


Electromagnetic Radiation

- Most subatomic particles behave as PARTICLES and obey the physics of waves.



Electromagnetic Radiation



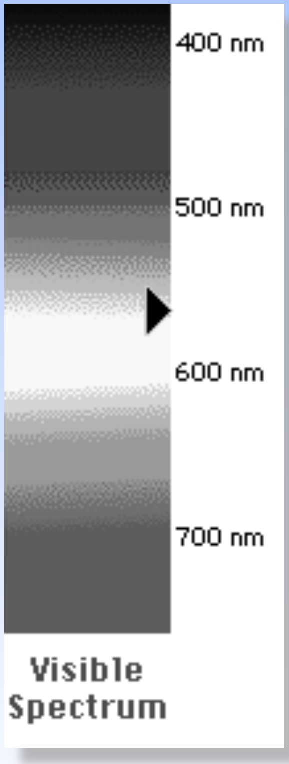
Electromagnetic Radiation

- Waves have a frequency
- Use the Greek letter "nu", ν, for frequency, and units are "cycles per sec"
- All radiation: $\lambda \cdot \nu = c$
  where c = velocity of light = 3.00×10^8 m/sec

Electromagnetic Spectrum

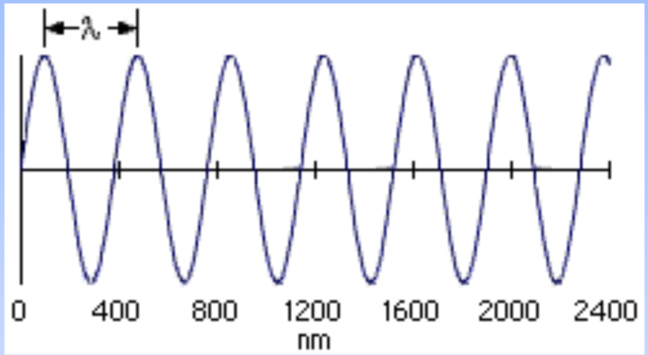
Long wavelength --> small frequency

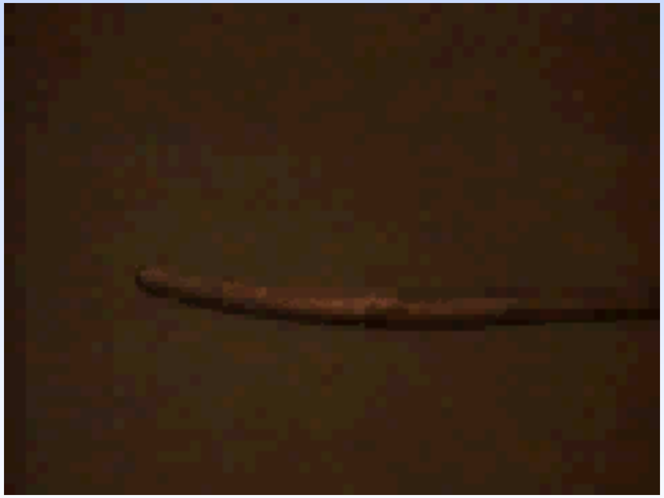
Short wavelength --> high frequency



increasing frequency

increasing wavelength





Electromagnetic Spectrum

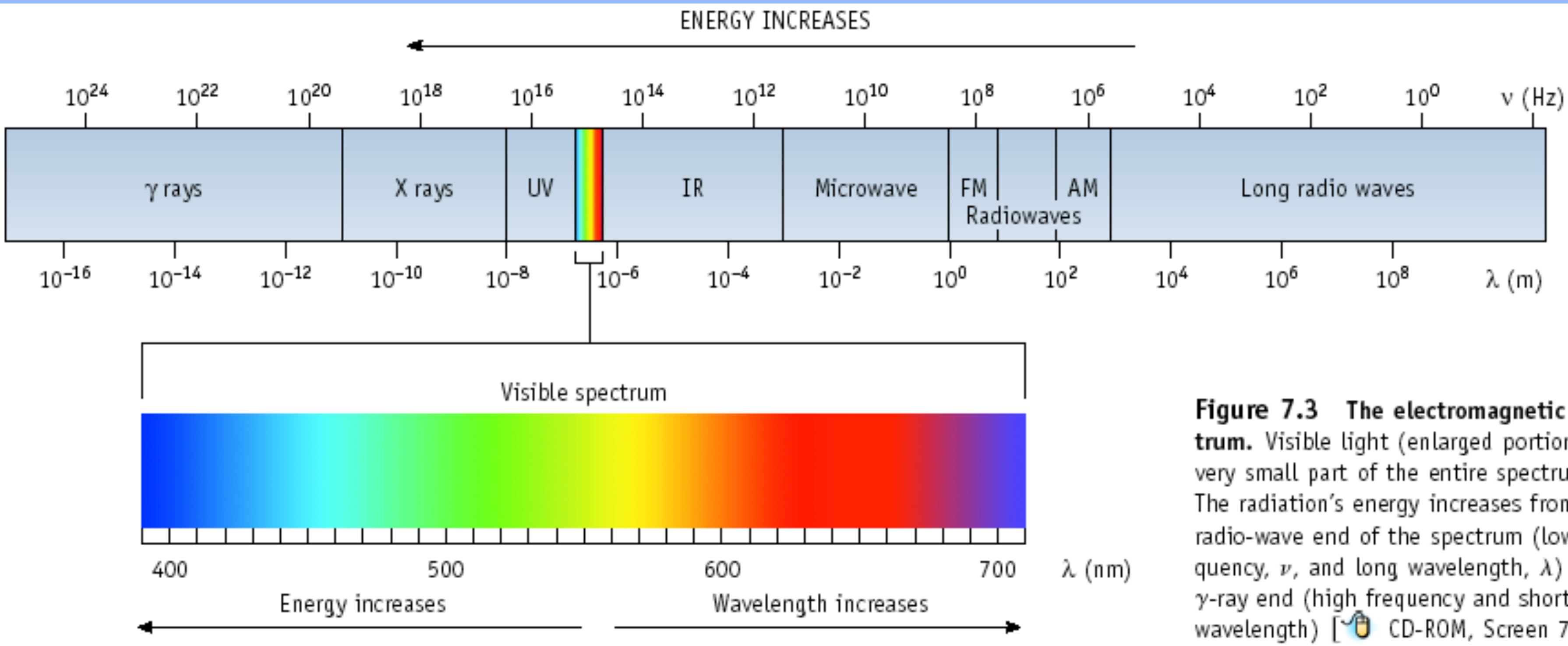


Figure 7.3 The electromagnetic spectrum. Visible light (enlarged portion) is a very small part of the entire spectrum. The radiation's energy increases from the radio-wave end of the spectrum (low frequency, ν, and long wavelength, λ) to the γ-ray end (high frequency and short wavelength) [CD-ROM, Screen 7.4].

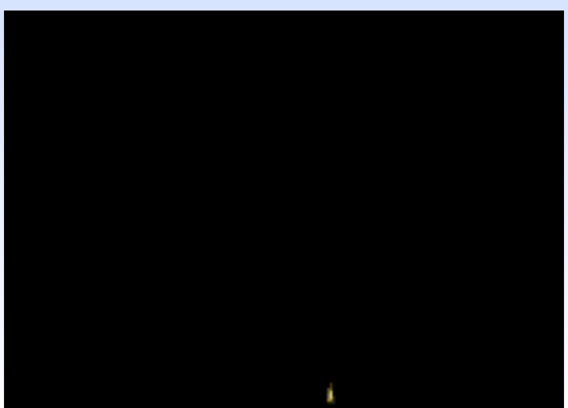
In increasing energy, ROY G BIV

Excited Gases & Atomic Structure

Electricity off.
Colorless gases.

Electricity on.
Excited electrons.

Gases such as neon are colorless. However, if electricity is passed through the gas, the atoms are excited, and the gas glows.



Atomic Line Emission Spectra and Niels Bohr

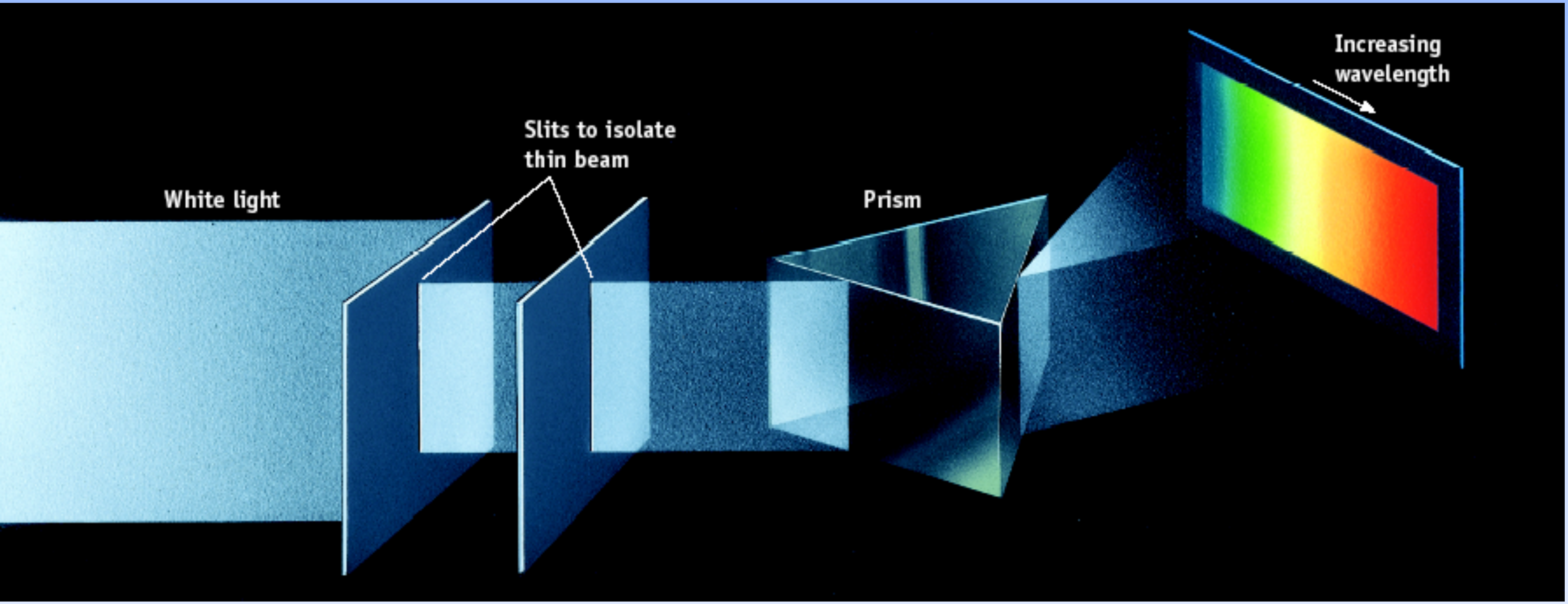
Niels Bohr

(1885-1962)

Bohr's greatest contribution to science was in building a simple model of the atom. It was based on an understanding of the **LINE EMISSION SPECTRA** of excited atoms.

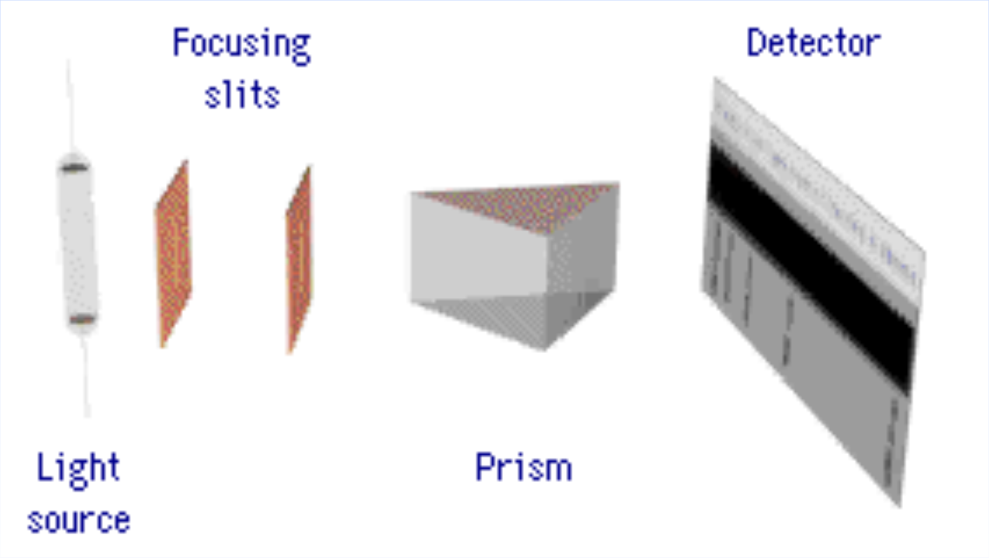
- Problem is that the model only works for H

Spectrum of White Light

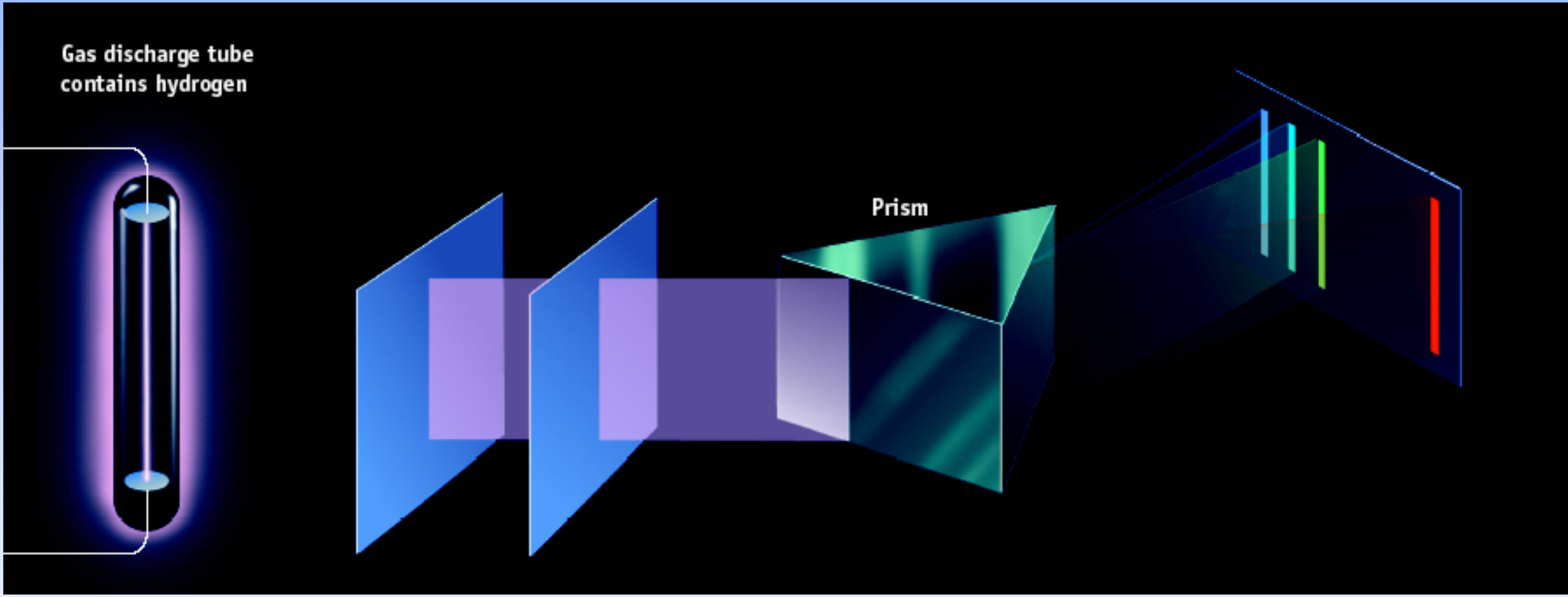


Line Emission Spectra of Excited Atoms

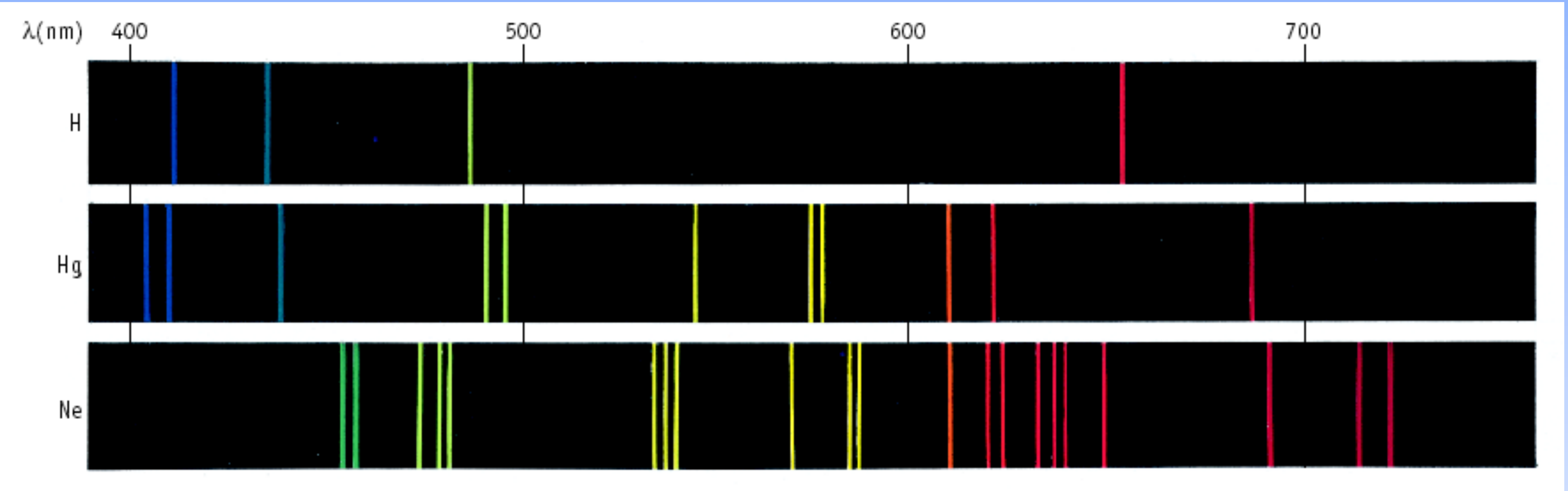
- Excited atoms emit light of only certain wavelengths
- The wavelengths of emitted light depend on the element.



Spectrum of Excited Hydrogen Gas



Line Spectra of Other Elements



The Electric Pickle

- Excited atoms can emit light.
- Here the solution in a pickle is excited electrically. The Na^+ ions in the pickle juice give off light characteristic of that element.

Atomic Spectra and Bohr

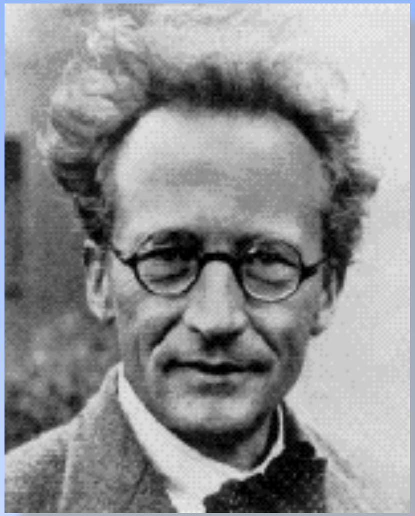
Bohr said classical view is wrong.

Need a new theory — now called **QUANTUM** or **WAVE MECHANICS**.

e- can only exist in certain discrete orbits

e- is restricted to **QUANTIZED** energy state (quanta = bundles of energy)

Quantum or Wave Mechanics



E. Schrodinger
1887-1961

Schrodinger applied idea of e- behaving as a wave to the problem of electrons in atoms.

He developed the **WAVE EQUATION**

Solution gives set of math expressions called **WAVE FUNCTIONS, Ψ**

Each describes an allowed energy state of an e-

Heisenberg Uncertainty Principle

W. Heisenberg
1901-1976

Problem of defining nature of electrons in atoms solved by W. Heisenberg.

Cannot simultaneously define the position and momentum (= m•v) of an electron.

We define e- energy exactly but accept limitation that we do not know exact position.

Arrangement of Electrons in Atoms

Electrons in atoms are arranged as

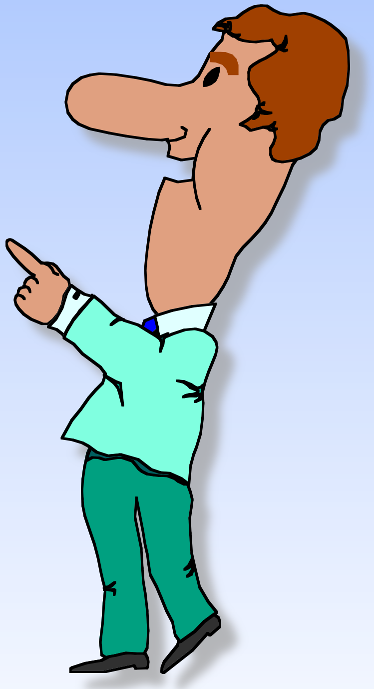
LEVELS (n)

↓

SUBLEVELS (l)

↓

ORBITALS (m_l)



QUANTUM NUMBERS

The **shape, size, and energy** of each orbital is a function of 3 quantum numbers which describe the location of an electron within an atom or ion

n (principal) ---> energy level

l (orbital) ---> shape of orbital

m_l (magnetic) ---> designates a particular suborbital

The fourth quantum number is not derived from the wave function

s (spin) ---> spin of the electron (clockwise or counterclockwise: ½ or – ½)

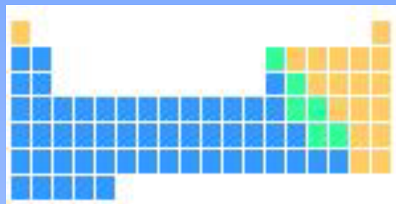
QUANTUM NUMBERS

So… if two electrons are in the same place at the same time, they must be repelling, so at least the spin quantum number is different!

The **Pauli Exclusion Principle** says that no two electrons within an atom (or ion) can have the same four quantum numbers.

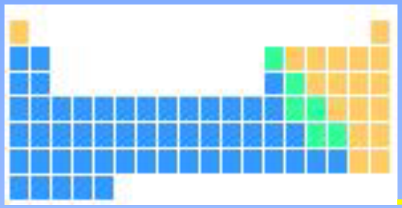
If two electrons are in the same energy level, the same sublevel, and the same orbital, they must repel.

Think of the 4 quantum numbers as the address of an electron… Country > State > City > Street

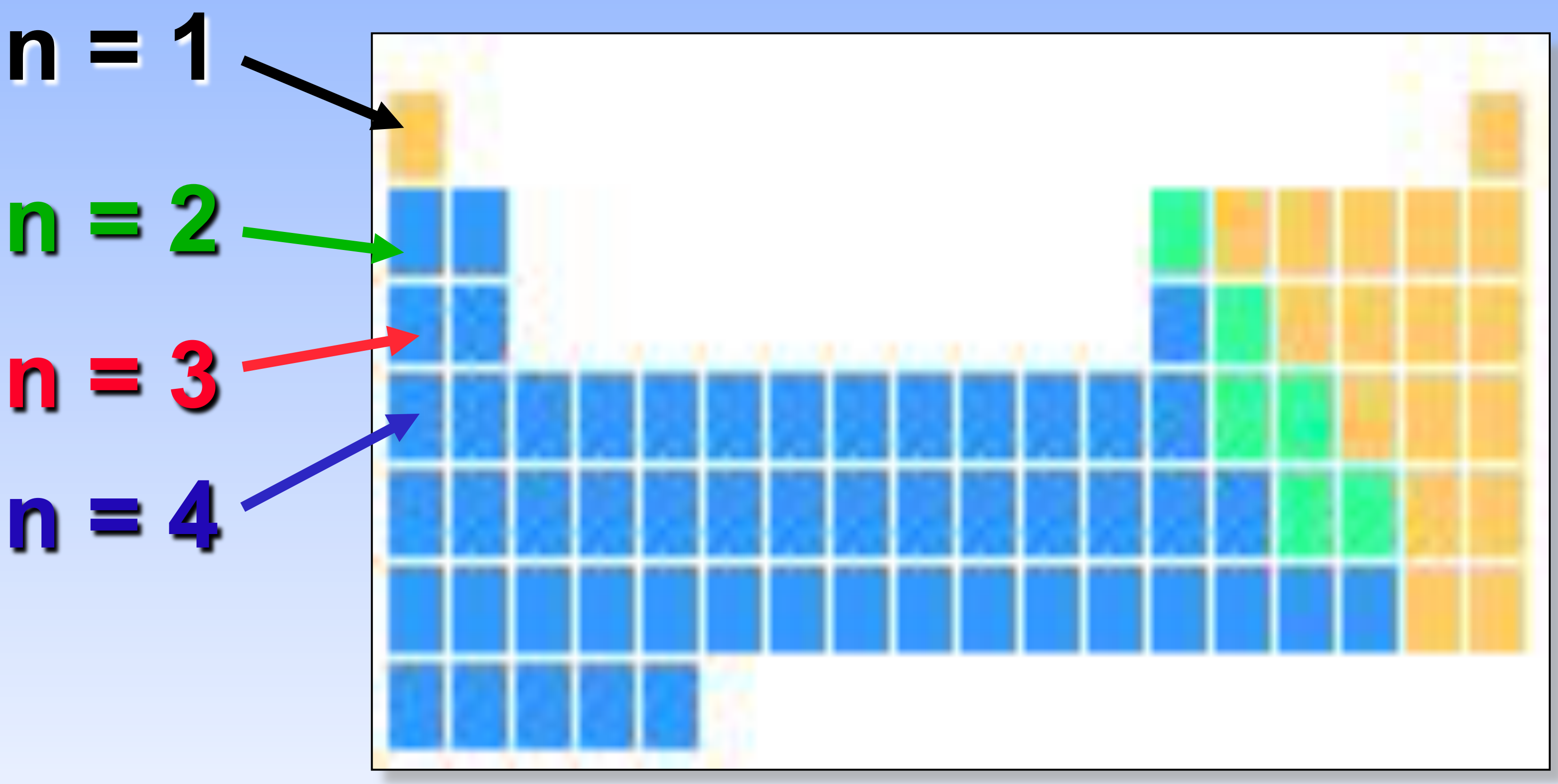


Energy Levels

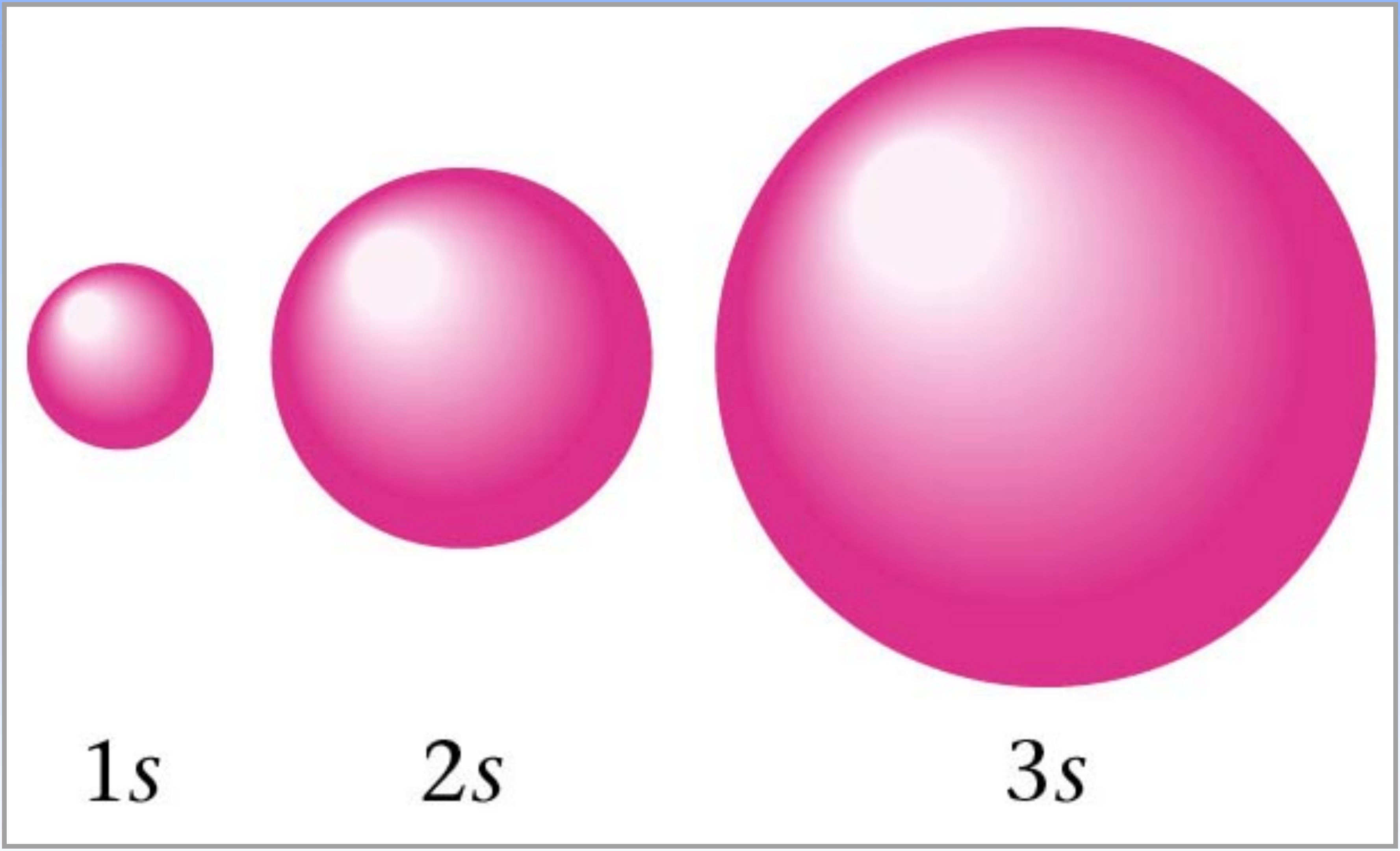
- Each energy level has a number called the **PRINCIPAL QUANTUM NUMBER, n**
- Currently n can be 1 thru 7, because there are 7 periods on the periodic table



Energy Levels



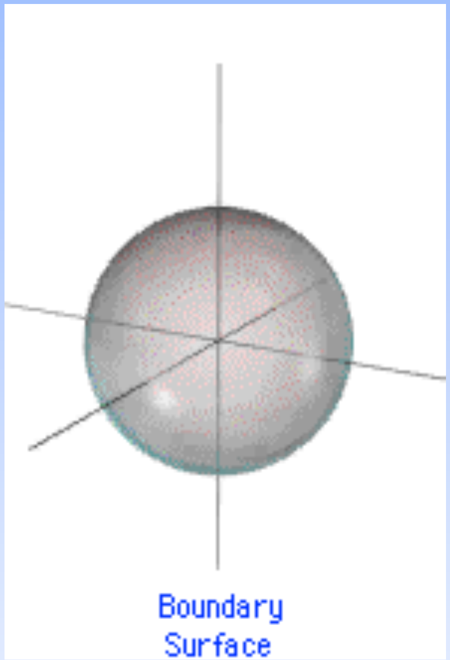
Relative sizes of the spherical 1*s*, 2*s*, and 3*s* orbitals of hydrogen.



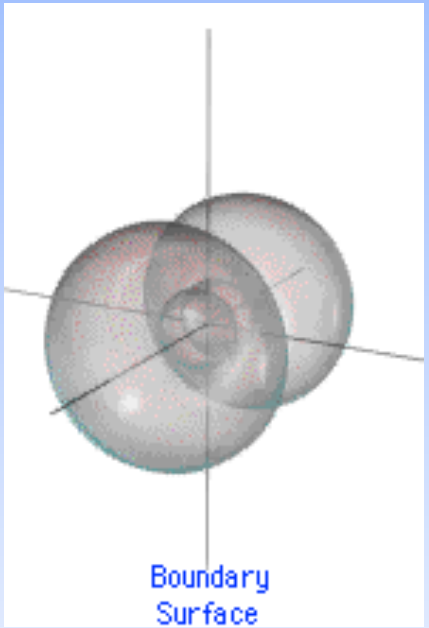
Types of Orbitals

- The most probable area to find these electrons takes on a shape
- So far, we have 4 shapes. They are named s, p, d, and f.
- No more than 2 e- assigned to an orbital – one spins clockwise, one spins counterclockwise

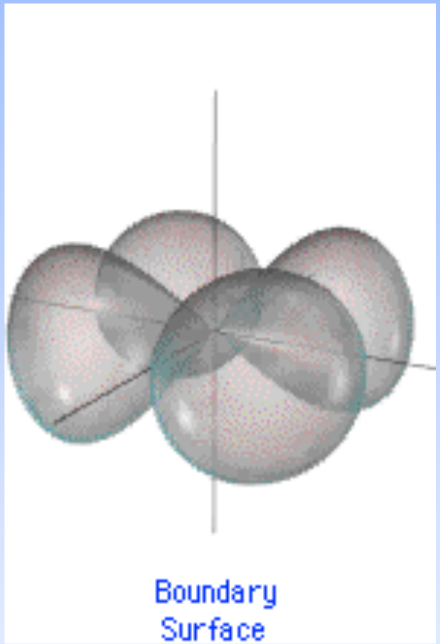
Types of Orbitals (l)



s orbital



p orbital



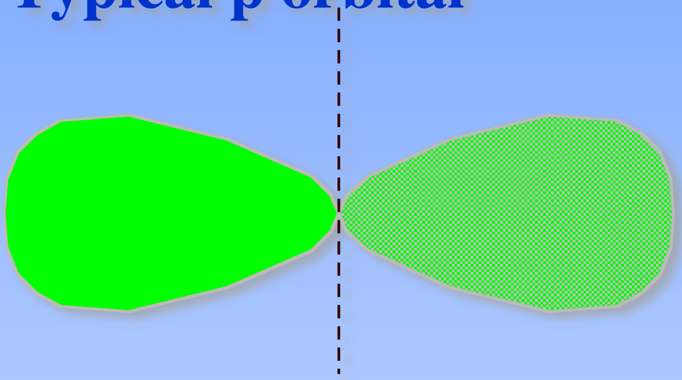
d orbital

p Orbitals

this is a p sublevel
with 3 orbitals

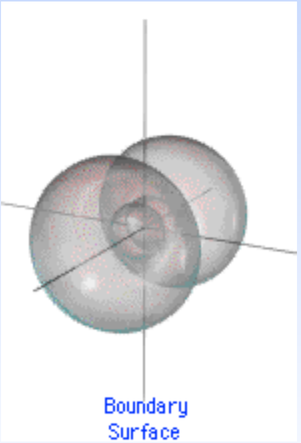
These are called x, y, and z

Typical p orbital



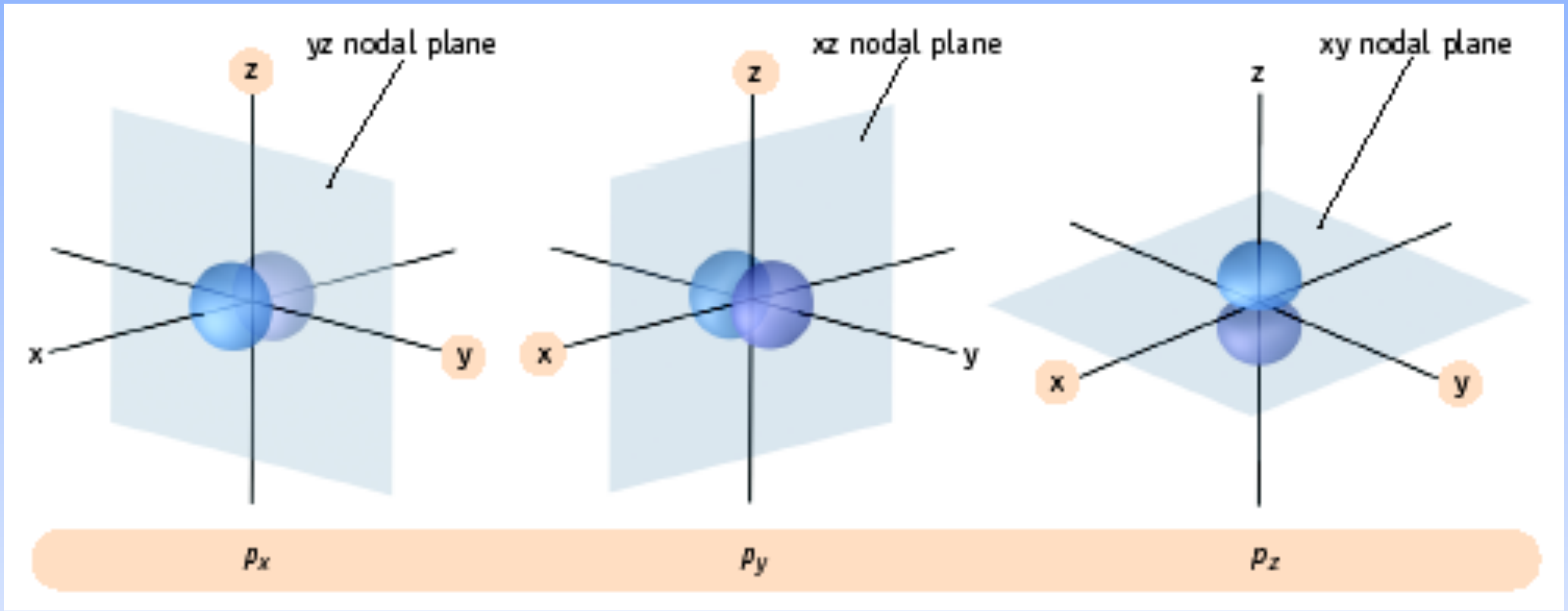
planar node

There is a **PLANAR NODE** thru the nucleus, which is an area of zero probability of finding an electron



$3p_y$ orbital

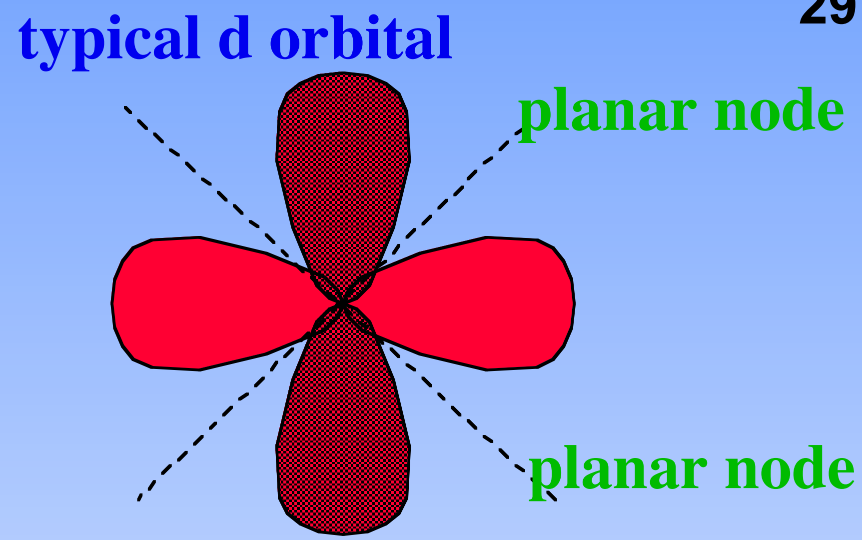
p Orbitals

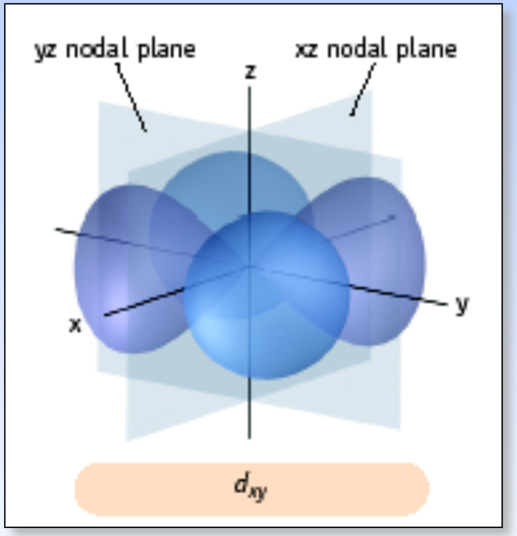


- The three p orbitals lie 90º apart in space

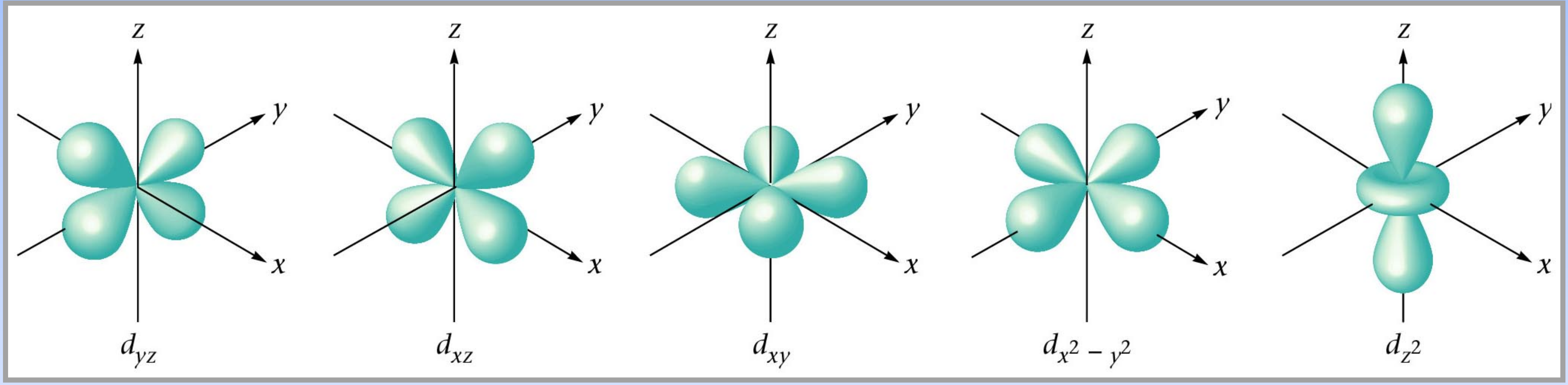
d Orbitals

- d sublevel has 5 orbitals



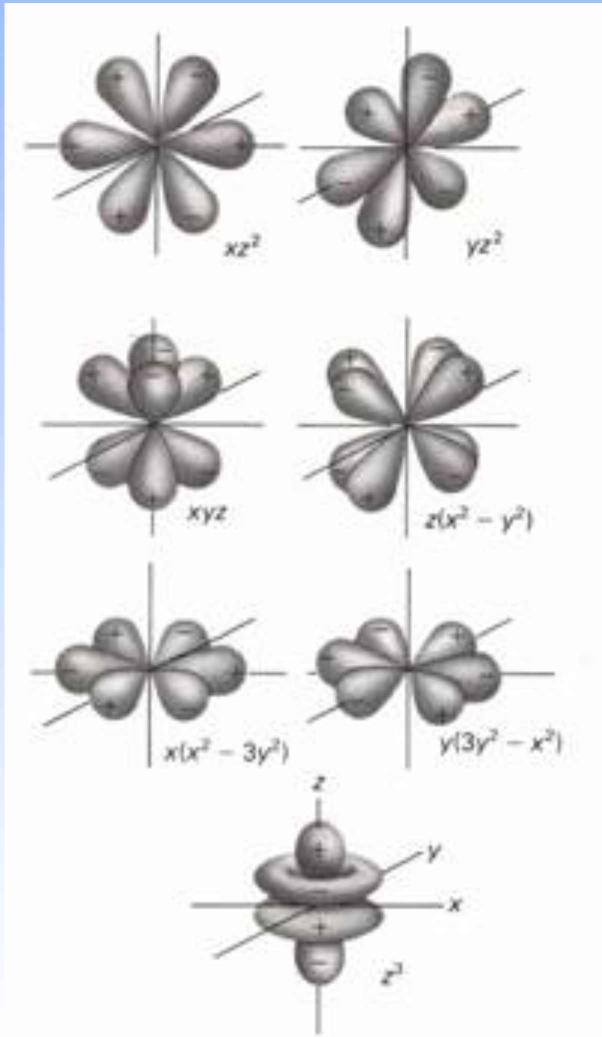


The shapes and labels of the five 3*d* orbitals.



f Orbitals

For l = 3,
---> f sublevel with 7 orbitals



Why are d and f orbitals always in lower energy levels?

- d and f orbitals require LARGE amounts of energy
- It's better (lower in energy) to skip a sublevel that requires a large amount of energy (d and f orbtials) for one in a higher level but lower energy

This is the reason for the diagonal rule! BE SURE TO FOLLOW THE ARROWS IN ORDER!

How many electrons can be in a sublevel?

Remember: A maximum of two electrons can be placed in an orbital.

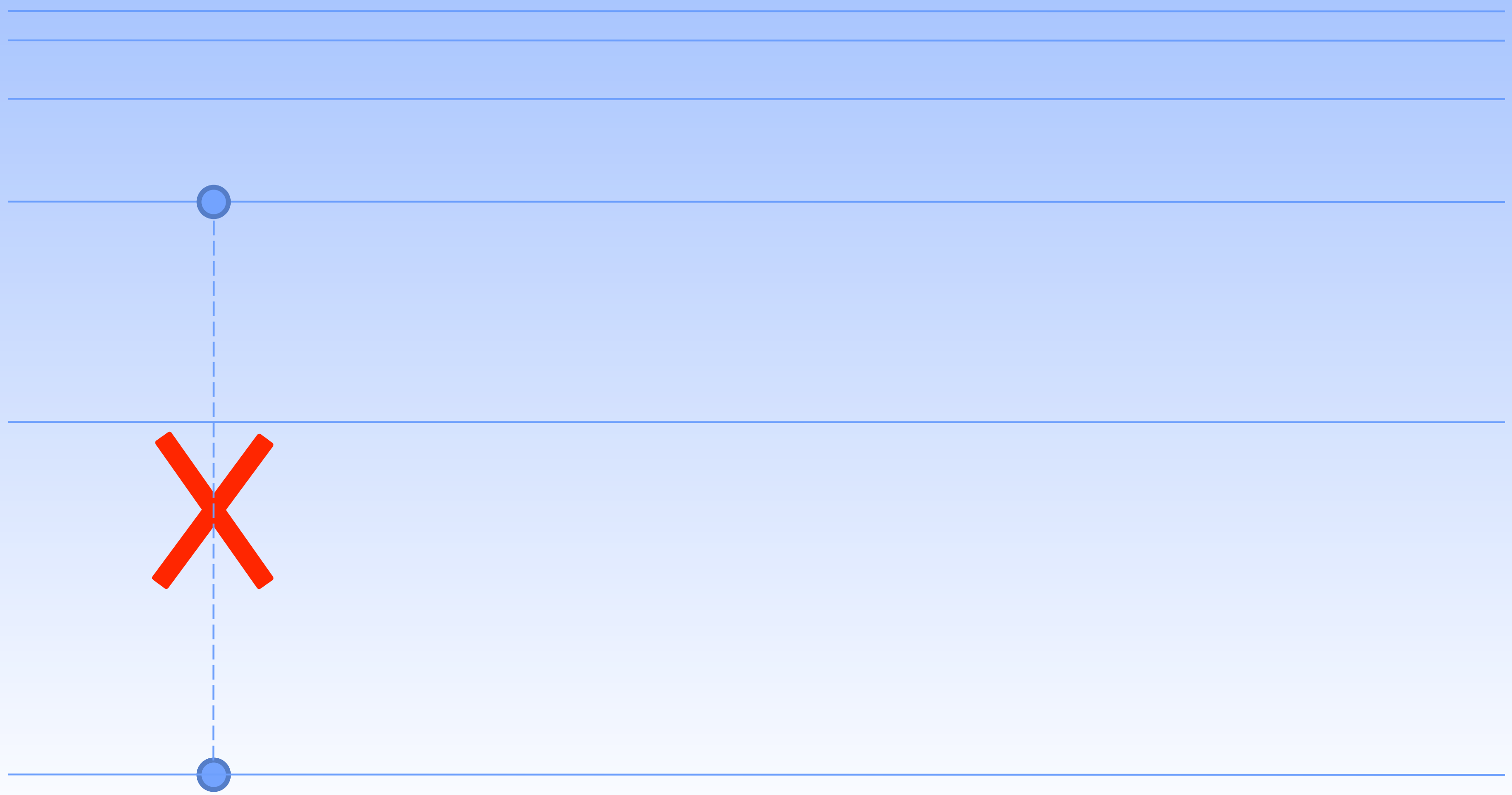
	s orbitals	p orbitals	d orbitals	f orbitals
Number of orbitals				
Number of electrons				

Writing Electron Configurations

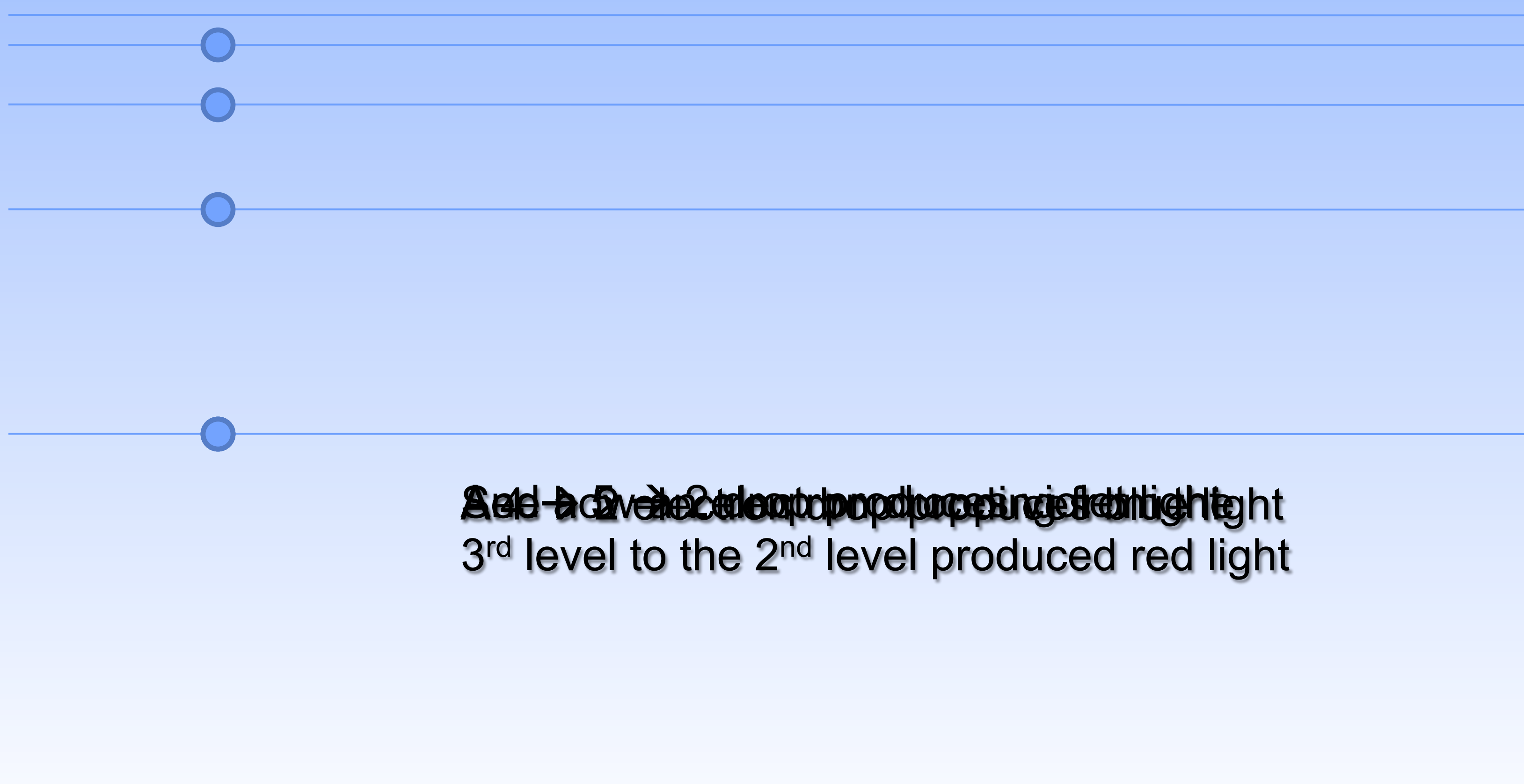
First let's review a little:
As we have learned, electrons exist in very specific energy levels.
And when these electrons absorb energy…
They get energized up to higher levels.
Actually, the jump to higher levels is not a gradual transition as was just shown.

It is a "quantum" jump, and looks more like this:

Quantum means it happens all at once – instantaneously – because the electron can never exist between levels – not even for a second.



Once it is at this higher level (excited state), it doesn't stay there long.
It quickly drops down to a lower level – again as a quantum leap – and as it does, it gives off a distinct band of light energy.
Also, notice how the electron doesn't have to drop all the way back down to the lowest level. It can get energized up to any level, and from there it can drop to any lower level. AND the different drops each produce different frequencies of light.



Electron Configurations

- Electron configurations tells us in which orbitals the electrons for an element are located.
- Three rules:
  - electrons fill orbitals starting with lowest n and moving upwards (Aufbau);
  - no two electrons can fill one orbital with the same spin (Pauli);
  - for degenerate orbitals, electrons fill each orbital singly before any orbital gets a second electron (Hund's rule).

Electron Configurations

A list of all the electrons in an atom (or ion)

- Must go in order (Aufbau principle)
- 2 electrons per orbital, maximum
- We need electron configurations so that we can determine the number of electrons in the outermost energy level. These are called *valence electrons*.
- The number of valence electrons determines how many and what this atom (or ion) can bond to in order to make a molecule

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}$… etc.

Electron Configurations

$2p^4$

Energy Level

Sublevel

Number of electrons in the sublevel

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}$… etc.

Electron Configuration

$1s^1$

row #
shell #
possibilities are 1-7
7 rows

subshell
possibilities are
s, p, d, or f
4 subshells

group #
valence e-
possibilities are:
s: 1 or 2
p: 1-6
d: 1-10
f: 1-14
Total e- should equal
Atomic #

What element has an electron configuration of $1s^1$?

Practice:

Ask these questions every time you have to write an electron configuration

- **Lithium:**

1. find the element on the periodic table — atomic # = 3
2. what is the period number? 2
3. how many shells? 2
4. what is the group number? 1
5. how many valence electrons? 1
6. what subshell(s) does Li have? s
7. what is the electron configuration? $1s^2\ 2s^1$

Practice:

Ask these questions every time you have to write an electron configuration

- **Boron:**

1. **find the element on the periodic table** atomic # = 5
2. **what is the row #?** 2
3. **how many shells?** 2
4. **what is the group #?** 3
5. **how many valence electrons?** 3
6. **what subshell(s) does B have?** p
7. **what is the electron configuration?** $1s^2\ 2s^2\ 2p^1$

Let's Try It!

- **Write the electron configuration for the following elements:**

  H

  Li

  N

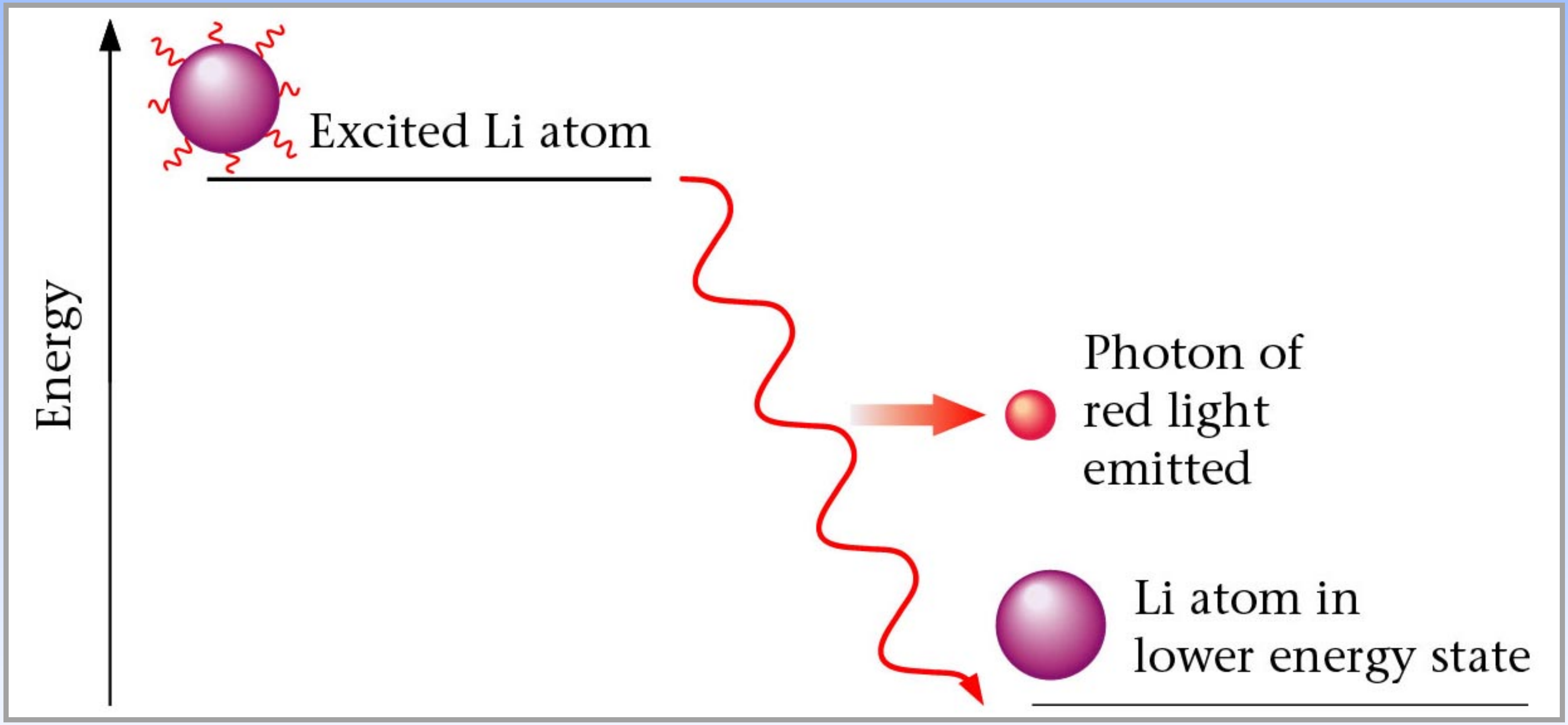
  Ne

  K

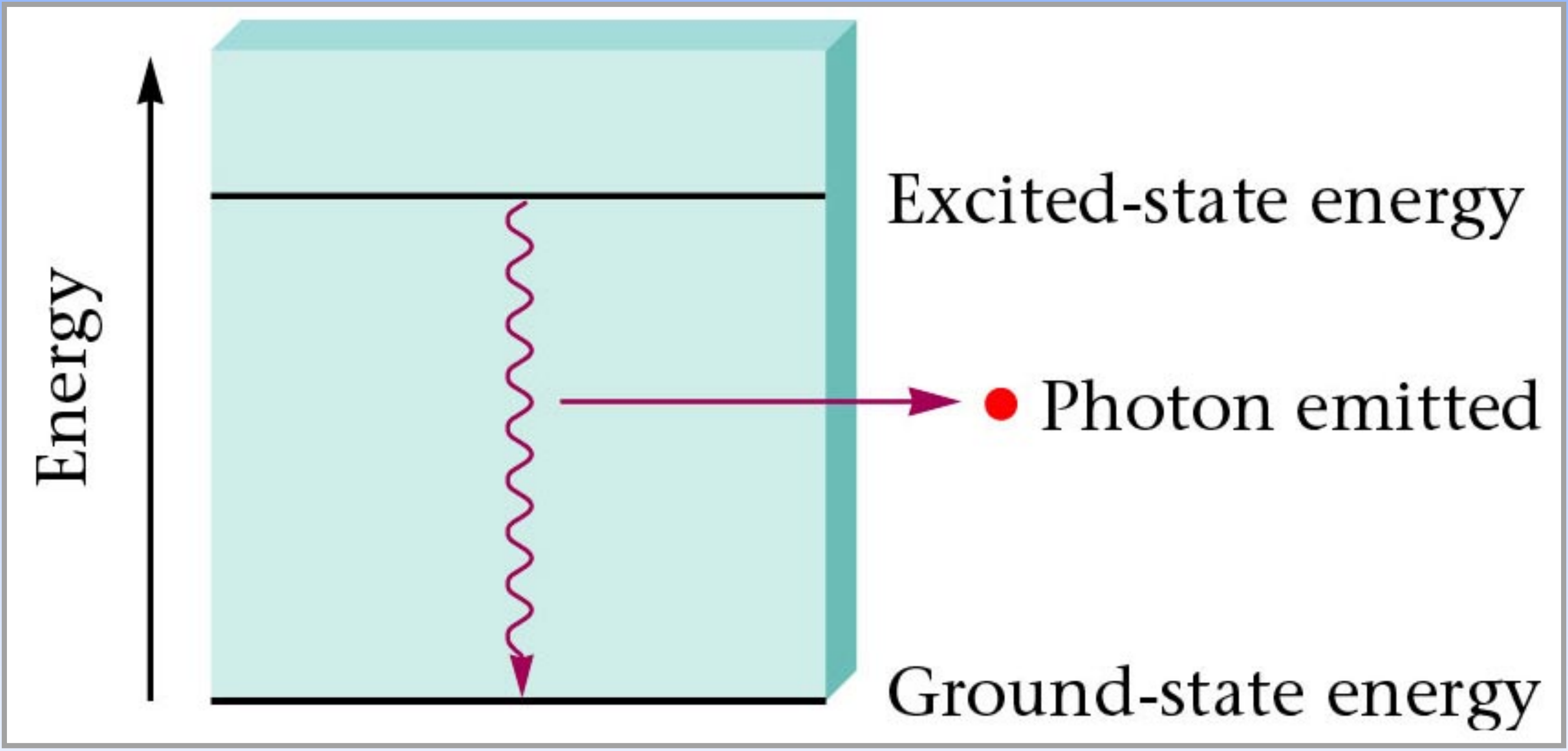
  Zn

  Pb

An excited lithium atom emitting a photon of red light to drop to a lower energy state.

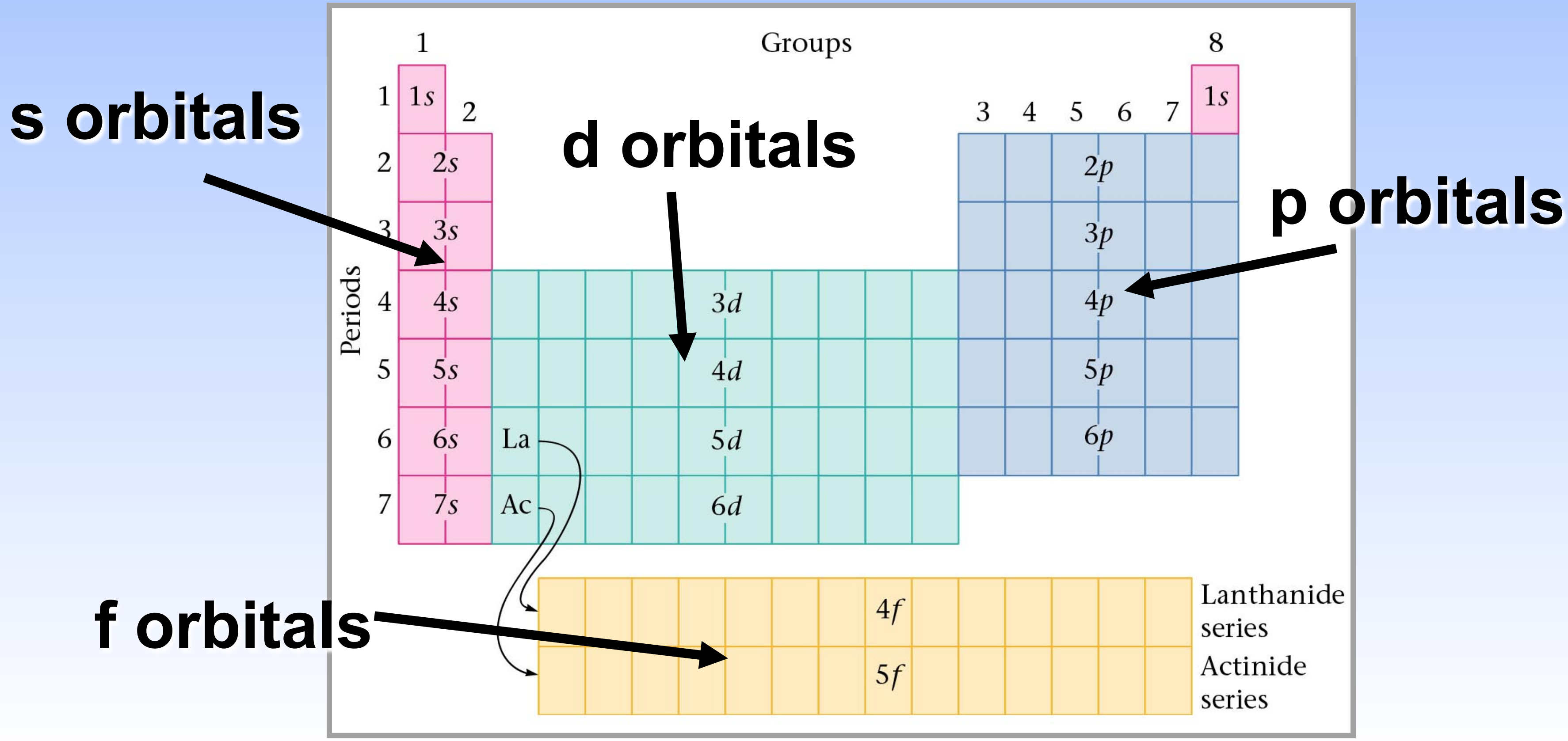


An excited H atom returns to a lower energy level.



Orbitals and the Periodic Table

- **Orbitals grouped in s, p, d, and f orbitals**
  (sharp, proximal, diffuse, and fundamental)



Shorthand Notation

- A way of abbreviating long electron configurations
- Since we are only concerned about the outermost electrons, we can skip to places we know are completely full (noble gases), and then finish the configuration

Shorthand Notation

- Step 1: It's the Showcase Showdown!

  Find the closest noble gas to the atom (or ion), WITHOUT GOING OVER the number of electrons in the atom (or ion). Write the noble gas in brackets [ ].
- Step 2: Find where to resume by finding the next energy level.
- Step 3: Resume the configuration until it's finished.

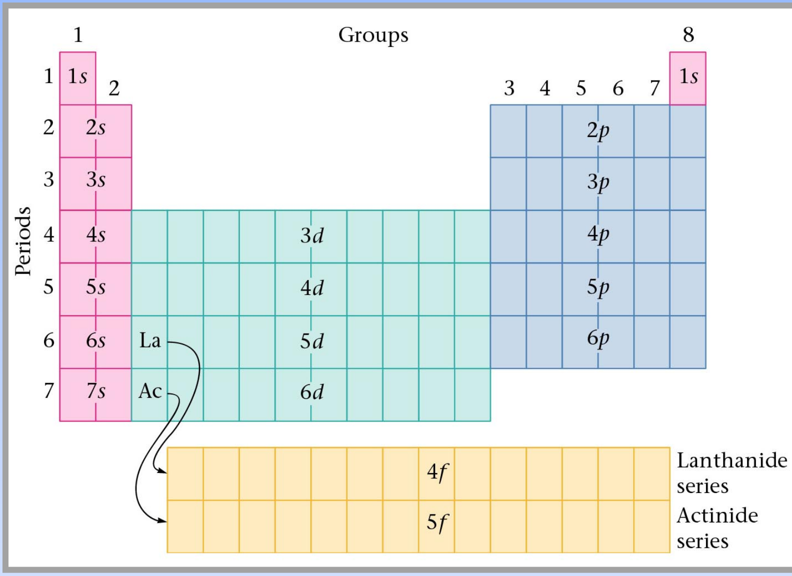
Shorthand Notation

- Chlorine
  - Longhand is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

  You can abbreviate the first 10 electrons with a noble gas, Neon. [Ne] replaces $1s^2\ 2s^2\ 2p^6$

  The next energy level after Neon is 3

  So you start at level 3 on the diagonal rule (all levels start with s) and finish the configuration by adding 7 more electrons to bring the total to 17



$[Ne]\ 3s^2\ 3p^5$

Practice Shorthand Notation

- Write the shorthand notation for each of the following atoms:

Cl

K

Ca

I

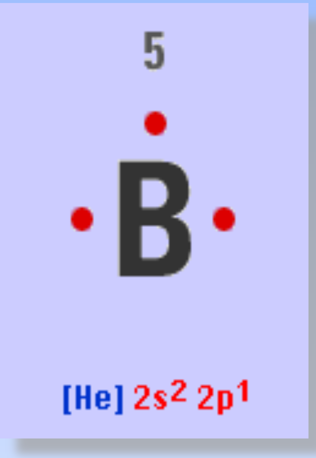
Bi

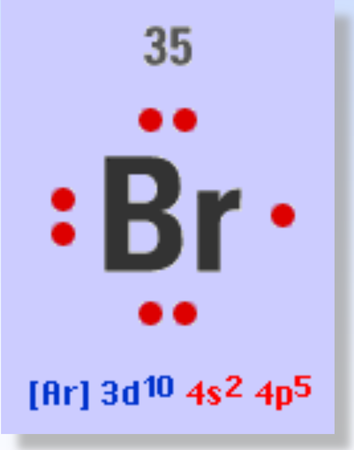
Valence Electrons

Electrons are divided between core and valence electrons

B $1s^2\ 2s^2\ 2p^1$

Core = [He] , valence = $2s^2\ 2p^1$





Br [Ar] $3d^{10}\ 4s^2\ 4p^5$

Core = [Ar] $3d^{10}$, valence = $4s^2\ 4p^5$

Keep an Eye On Those Ions!

- **Electrons are lost or gained like they always are with ions… negative ions have gained electrons, positive ions have lost electrons**
- **The electrons that are lost or gained should be added/removed from the *highest energy level* (not the highest orbital in energy!)**

Keep an Eye On Those Ions!

- Tin

__Atom:__ [Kr] $5s^2$ $4d^{10}$ $5p^2$

__Sn^{+4} ion:__ [Kr] $4d^{10}$

__Sn^{+2} ion:__ [Kr] $5s^2$ $4d^{10}$

Note that the electrons came out of the highest energy level, not the highest energy orbital!

Keep an Eye On Those Ions!

- Bromine

Atom: [Ar] $4s^2 3d^{10} 4p^5$

Br^- ion: [Ar] $4s^2 3d^{10} 4p^6$

Note that the electrons went into the highest energy level, not the highest energy orbital!

Try Some Ions!

- Write the longhand notation for these:

F^-

Li^+

Mg^{+2}

- Write the shorthand notation for these:

Br^-

Ba^{+2}

Al^{+3}

Exceptions to the Aufbau Principle

- Remember d and f orbitals require LARGE amounts of energy
- If we can't fill these sublevels, then the next best thing is to be HALF full (one electron in each orbital in the sublevel)
- There are many exceptions, but the most common ones are

d^4 and d^9

For the purposes of this class, we are going to assume that ALL atoms (or ions) that end in d^4 or d^9 are exceptions to the rule. This may or may not be true, it just depends on the atom.

Exceptions to the Aufbau Principle

d^4 is one electron short of being HALF full

In order to become more stable (require less energy), one of the *closest s* electrons will actually go into the d, making it d^5 instead of d^4.

For example: Cr would be [Ar] $4s^2$ $3d^4$, but since this ends *exactly* with a d^4 it is an exception to the rule. Thus, Cr should be [Ar] $4s^1$ $3d^5$.

Procedure: Find the closest s orbital. Steal one electron from it, and add it to the d.

Exceptions to the Aufbau Principle

- OK, so this helps the d, but what about the poor s orbital that loses an electron?

- Remember, half full is good… and when an s loses 1, it too becomes half full!

- So… having the s half full and the d half full is usually lower in energy than having the s full and the d to have one empty orbital.

Exceptions to the Aufbau Principle

d^9 is one electron short of being full

Just like d^4, one of the *closest s* electrons will go into the d, this time making it d^{10} instead of d^9.

For example: Au would be [Xe] $6s^2$ $4f^{14}$ $5d^9$, but since this ends *exactly* with a d^9 it is an exception to the rule. Thus, Au should be [Xe] $6s^1$ $4f^{14}$ $5d^{10}$.

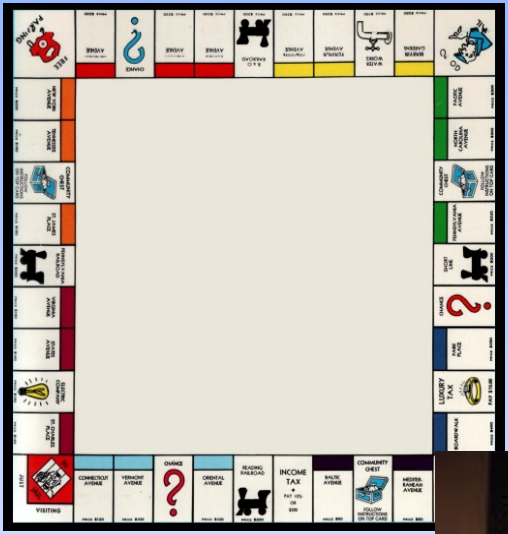
Procedure: Same as before! Find the closest s orbital. Steal one electron from it, and add it to the d.

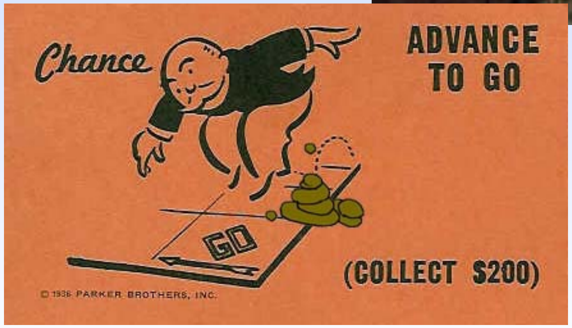
Orbital Diagrams

- Graphical representation of an electron configuration
- One arrow represents one electron
- Shows spin and which orbital within a sublevel
- Same rules as before (Aufbau principle, d^4 and d^9 exceptions, two electrons in each orbital, etc. etc.)

Orbital Diagrams

- One additional rule: Hund's Rule
  - In orbitals of EQUAL ENERGY (p, d, and f), place one electron in each orbital before making any pairs
  - All single electrons must spin the same way
- I nickname this rule the "Monopoly Rule"
- In Monopoly, you have to build houses EVENLY. You can not put 2 houses on a property until all the properties have at least 1 house.



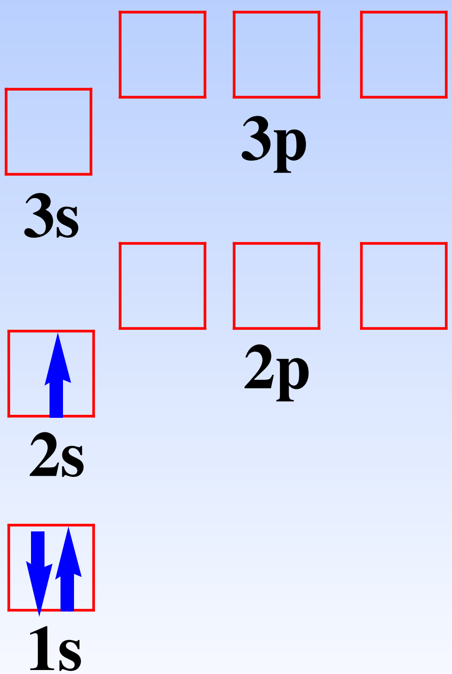


Lithium

Group 1A

Atomic number = 3

$1s^2 2s^1$ ---> 3 total electrons



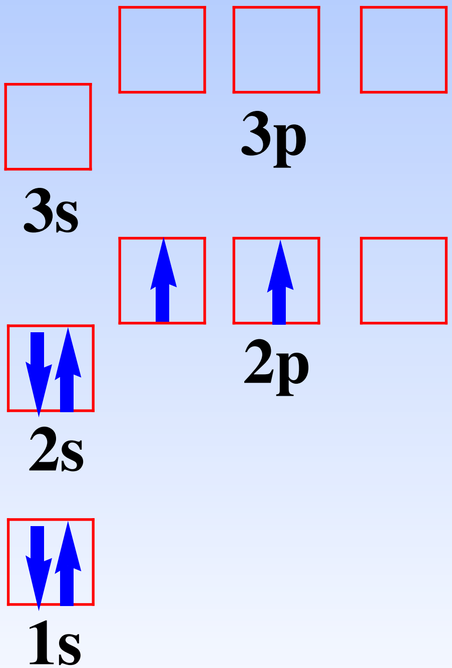
Carbon

Group 4A

Atomic number = 6

$1s^2\,2s^2\,2p^2$ --->

6 total electrons



Here we see for the first time HUND'S RULE. When placing electrons in a set of orbitals having the same energy, we place them singly as long as possible.

Draw these orbital diagrams!

- Oxygen (O)
- Chromium (Cr)
- Mercury (Hg)

The End !!!!!!!!!!!!!!!!!!!!!