

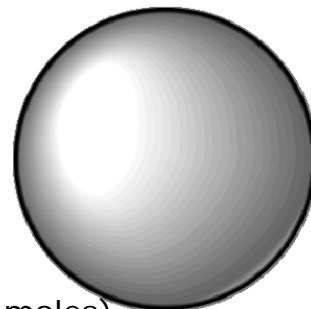
# Atomic Theory

## Early models

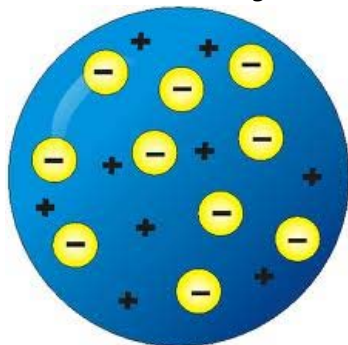
- Ancient Greece → Late 18<sup>th</sup> century
- 4 elements – Air, Water, Wind, Fire: Matter is made up in different combinations of these 4 elements.
- First “atom” proposed by Democritus (Greek) smallest unit that cannot be broken down

## Atoms – Billiard Ball model

- Early 19<sup>th</sup> century
- J. Dalton (1806) *law of multiple proportions* (combine in small integers)
- Atoms – smallest particles: hard sphere like balls
- A. Avogadro’s law (1811) (equal volumes of gases ∴ equal moles)
- Not really accepted until late 19<sup>th</sup> century



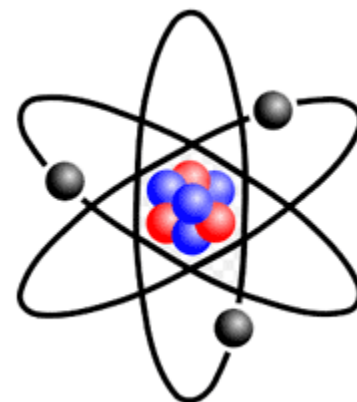
## Discovery of electrons – Plum Pudding model



- Late 19<sup>th</sup> century
- J.J. Thomson (1897) experiments with cathode ray tubes – discovers electrons – charged particles smaller than atoms
- R. Millikan – oil drop experiment (1909) figures out mass and charge of  $e^-$
- Plum pudding model: Mass of positive “goo” with electrons shoved in like raisins in plum pudding

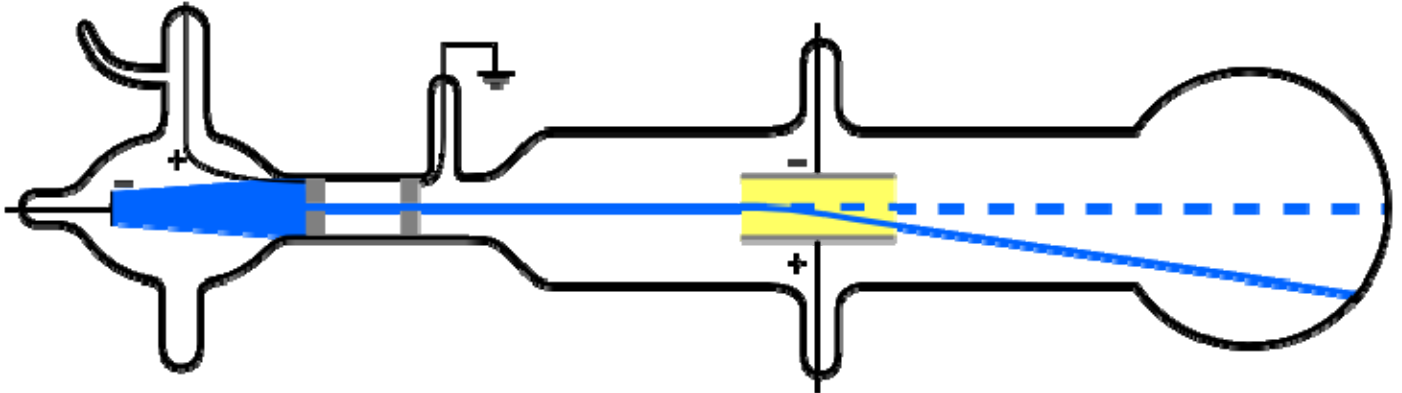
## Nucleus – Planetary model

- Early 20<sup>th</sup> century
- E. Rutherford’s Gold foil experiment (1909) most of the mass and positive charge of an atom is concentrated in a very small fraction of its volume
- Matter is mostly space
- Nucleus: dense mass in the middle, and electrons orbit like planets
- Neutron: Nucleus mass couldn’t be just from protons, had to be another, non charged, species (J. Chadwick discovered ~ 1930)

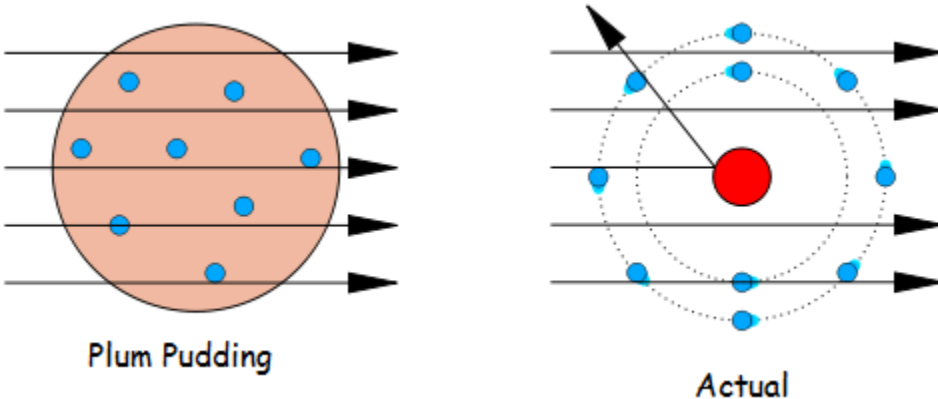


## Experiments (just a sampling)

- **Thomson – cathode rays**
- Found that rays bent towards the positive end, so these rays had to be negative
- Also found that magnets effected the ray in similar ways



- **Rutherford – Gold foil experiment**
- Shot alpha particles at gold foil, in theory they should go right through, but some shot back or were dramatically deflected



## Electrons, energy levels, and the Quantum Mechanical model

- mid 20<sup>th</sup> century
- Problem with Rutherford's model is that  $e^-$  and  $p^+$  should attract and  $e^-$  will "fall" into the nucleus.
- M. Planck and A. Einstein: electrons move up and down in simple levels, emitting EM energy in discrete packets called "quanta"
- E. Schrodinger: mathematical probabilities of where electrons can exist → shapes (s,p,d,f... orbitals) – will talk about later

## Isotopes

One of the interesting things to come out of Rutherford's experiments was that there was a fairly massive (~ 1 amu) particle that had no charge found in the nucleus... Neutrons

An Isotope: chemical species with the same number of protons (same element) but with a different number of neutrons.

Notation:  $^{12}_6\text{C}$  vs  $^{13}_6\text{C}$

**Ex.**  $^{13}_6\text{C}$  The bottom number is the protons; the top number is the overall mass (neutrons + protons)

This isotope has **6 protons** (making it Carbon) and  $13 - 6 =$  **7 neutrons**.

Also, because it has no charge it has **6 electrons**

**Ex.**  $^{41}_{20}\text{Ca}^{2+}$  **Protons = 20, Electrons = 18, Neutrons = 21**

## Atomic Mass Calculations

Recall: Atomic mass is the weighted average of all isotopes of an element

**Ex.** Chlorine is a mixture of 75.77% Chlorine 35 24.23% Chlorine 37  
What's the atomic mass?

$$\text{one mole: } \frac{75.77}{100} \times 35\text{g} + \frac{24.23}{100} \times 37\text{g} = 35.5 \text{ g}$$

**Ex.** What's the atomic mass of molybdenum?

$$^{92}_{42}\text{Mo} = 15.8\% \quad ^{94}_{42}\text{Mo} = 9.0\% \quad ^{95}_{42}\text{Mo} = 15.7\%$$

$$^{96}_{42}\text{Mo} = 16.5\% \quad ^{97}_{42}\text{Mo} = 9.5\% \quad ^{98}_{42}\text{Mo} = 23.8\%$$

$$^{100}_{42}\text{Mo} = 9.6\%$$

**A: 95.9 amu (or g/mol)**

## Energy and Electrons

Understanding the behavior of electrons in atoms is essential for understanding how atoms react with other atoms to form ions or molecules

Electrons can be thought of as particles or as waves (E. Schrodinger)

The modern model of the atom has electrons described as occupying discrete energy levels. To understand these levels we first need to look at waves and light.

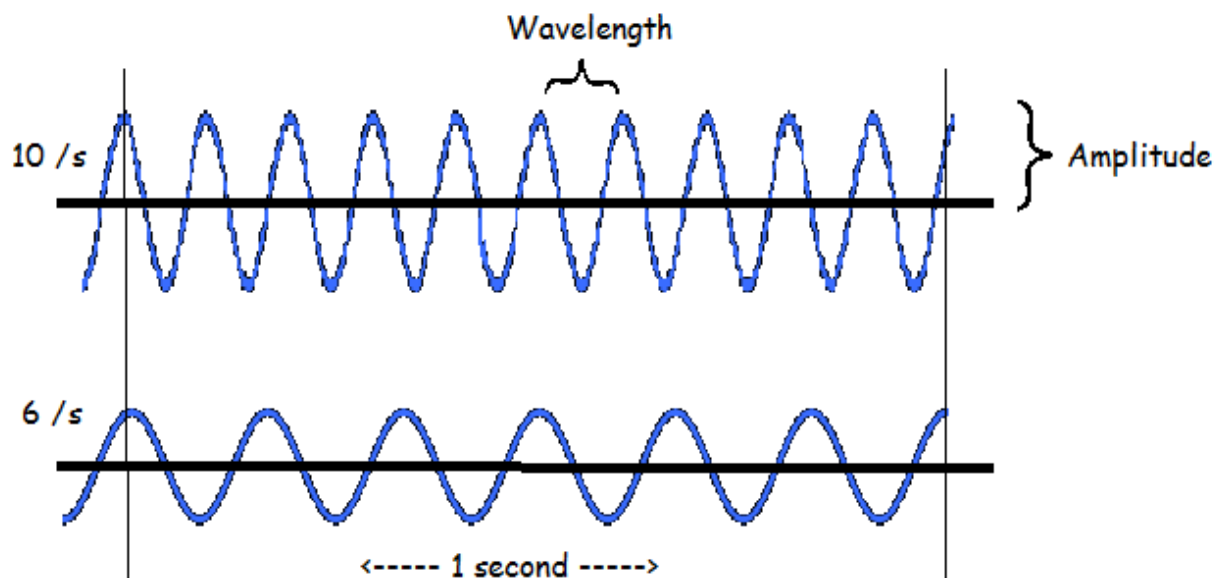
### Waves

A wave is a disturbance that transfers energy from one point to another in a medium

$\nu$  - frequency: the number of waves that pass a point in a unit of time (measured in Hz,  $s^{-1}$ , 1/s etc...)

$\lambda$  - wavelength: the distance between similar points of adjacent waves, ie. crest to crest (distance, so measured in m or nm)

**A** – amplitude: the distance from the crest to the midline



## Light

Light is composed of waves which can be characterized by their wavelength and frequency. The energy of light comes in discrete packages we call "*photons*"

The energy of a photon can be described by the equation:

$$E = hf$$
 Where  $E$  = energy measured in joules

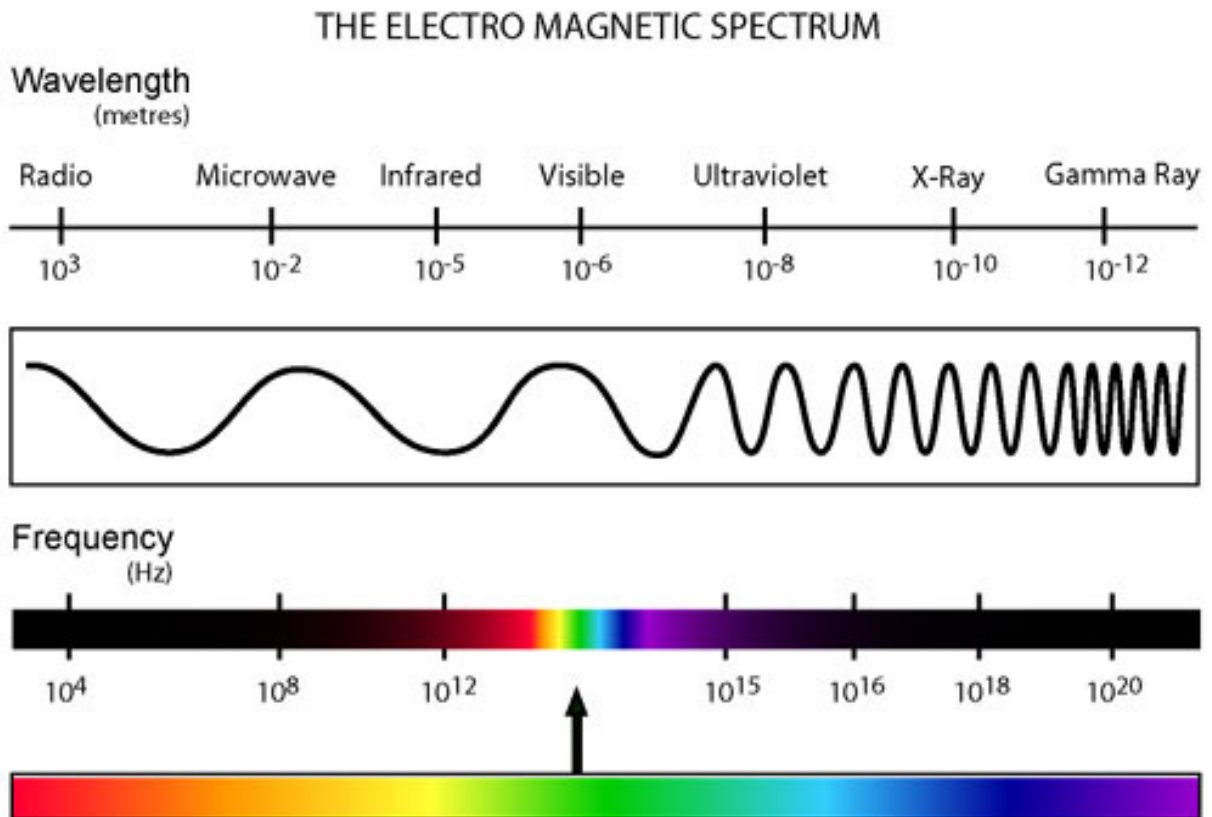
$h$  – Planck's constant: a fundamental constant ( $6.626 \times 10^{-34}$  J·s)

We can also make use of the relationship between frequency & wavelength:

$$c = \lambda f$$

$c$  – speed of light: a fundamental constant, nothing can go faster.  
( $\sim 3.0 \times 10^8$  m/s)

## EM spectrum



## Electrons

Scientists measure the wavelength of light given off by different elements when they are electrically excited. Only certain wavelengths of light are emitted and these correspond to the energy given off when the electrons move from one energy level to another. The energy of an electron changes by certain fixed values only (quanta) thus we called it *quantized*.

In 1885 Balmer described the energy given off by hydrogen gas using the equation:

$$E = \left[ \frac{1}{2^2} - \frac{1}{n^2} \right] \cdot K$$

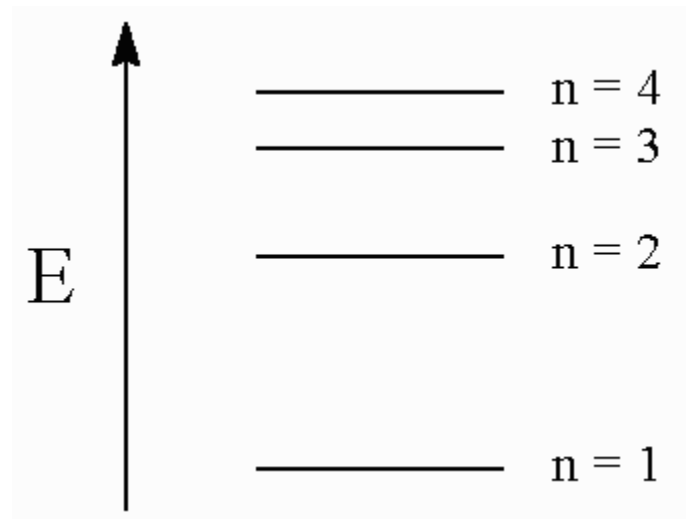
$n = 3, 4, 5\dots$  (integer  $> 2$ ), and

$K$  is some constant (irrelevant at this point)

$E$  = the energy of spectral lines, corresponding to electronic transitions in H

As  $n$  increases,  $E$  also increases (to ionization). Unfortunately this only worked for hydrogen and not for more complex atoms

Bohr proposed that there were discrete energy levels and that the electron moved up and down energy levels like climbing a staircase. When an electron absorbs energy it moves up one or more steps, but cannot stop between steps. The electron can emit energy when it moves down one or more steps, as light. The energy of the light emitted is quantized, meaning only certain frequencies of light can be observed: spectral lines.



He suggested that electrons themselves are quantized, that they exist only in certain, definite energy states, now called energy levels

## Quantum Orbitals

The energy levels of the electrons are represented by quantum numbers. The principal quantum number,  $n$ , represents the energy level and can be any whole number (1,2,3,4,5...)

Each energy level contains orbitals (places of increased probability of finding an electron) the number of orbitals increases as the principal quantum number increases. The number of different types of orbitals is equal to the principal quantum number. The orbitals are given the letters (in order)

s, p, d, f, g, h (although we're only going to use s, p and d, and maybe f)

Each orbital can only contain 2 electrons (Pauli exclusion principle)

There is 1 s orbital (2 electrons) -  $n = 1, 2, 3, 4, 5...$

There are 3 p orbitals (6 electrons) -  $n = 2, 3, 4, 5...$

There are 5 d orbitals (10 electrons) -  $n = 3, 4, 5...$

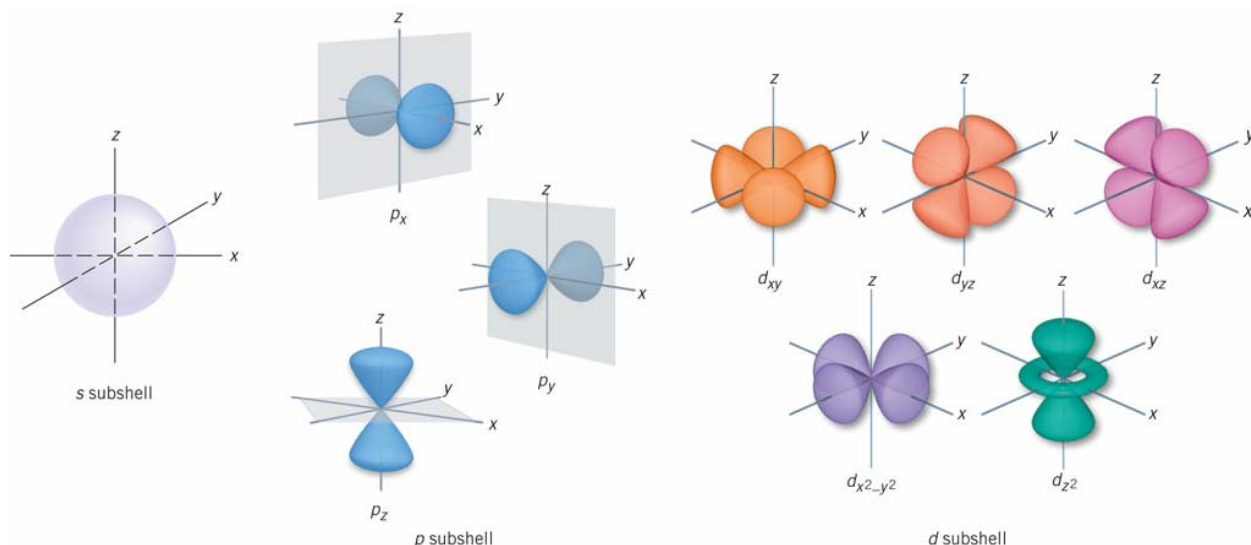
There are 7 f orbitals (14 electrons) -  $n = 4, 5...$

Even though there are 3 p orbitals (and 5 d, and 7 f, etc...) each orbital is at the same energy level (degenerate)

Electrons would rather be separate in an orbital than paired up (Hund's Rule) so if there is an empty orbital, fill it first.

## Orbital shapes

Orbitals are 3D, graphical representation of regions of high probability of finding the electrons of an atom around a nucleus.



## ***Energy configurations***

The orbitals fill in the following order:

1s (2) → 2s (2) → 2p (6) → 3s (2) → 3p (6) → 4s (2) → 3d (10) → 4p (6)  
etc...

**Ex.** What is the electron configuration for potassium (K)

K has 19 electrons, so the configuration is:  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

For an element (like K above) the #  $e^-$  = # $p^+$  (from the PT)

Ions: positive ions have lost electrons, negative ions have gained electrons

Always remove from the highest level that is populated, and add to the lowest level unpopulated

**Ex.** What is the electron configuration for Cu,  $Cu^+$  (copper is # 29)

Cu:  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^9$

$Cu^+$ :  $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$

Ground State: no excited  $e^-$ , all electrons in lowest possible orbitals

Excited State: Higher in energy, some electron(s) in higher energy level.



## Core Notation

Noble gases are neutral and stable – have a filled outermost orbital (recall: stable octet, octet rule) Once we reach the level of a noble gas we can use that as a “short hand”

**Ex.**  $K = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$  but the  $\{1s^2 2s^2 2p^6 3s^2 3p^6\}$  part is all the same as Argon (Ar) so we can simplify it as = [Ar]. Potassium would therefore be: **[Ar]4s<sup>1</sup>**

Ions usually form to create filled outer orbitals, either by losing or gaining a few electrons, they're trying to get more “noble gas-like”. Notice that when potassium loses an electron, and when chlorine gains an electron, they have the same electron configuration as argon = STABLE. When two species have the same electronic configuration we call them *isoelectronic*

## D - Exceptions

When d orbitals are either filled or half filled their orbital energy level can be lowered to less than the preceding s orbital. So our copper orbitals above actually look like:

