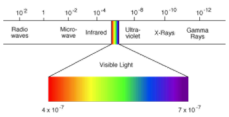
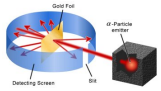
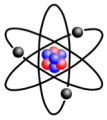
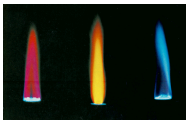
INTRO AND BACKGROUND:

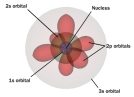
Atomic Structure

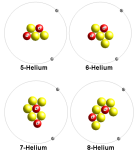






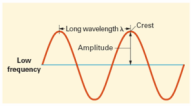


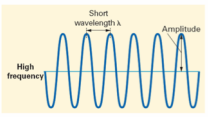




Light

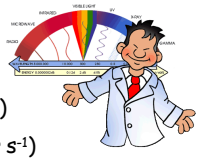
- Study of light by Newton helped lead to the quantum mechanical model
- All light exhibits **WAVE** properties
  - -**AMPLITUDE**: height of a wave
  - -**WAVELENGTH**: distance between waves (m)
  - -**FREQUENCY**: # of wave cycles to pass a point over a unit of time (hertz, Hz or s^{-1})
- All light (in a vacuum) moves at the speed of light… 3.00 x 10^8 m/s (**c**)





Electromagnetic Spectrum

- 7 Regions
- Ranked with respect to their wavelengths
- As the wavelengths become longer the frequency decreases (**INVERSE** relationship)
- Equation to explain this: $c = \lambda \nu$
  - c = **speed of light** (3 x 10^8 m/s)
  - λ = **wavelength** (measured in meters)
  - ν = **frequency** (measured in hertz or s^{-1})



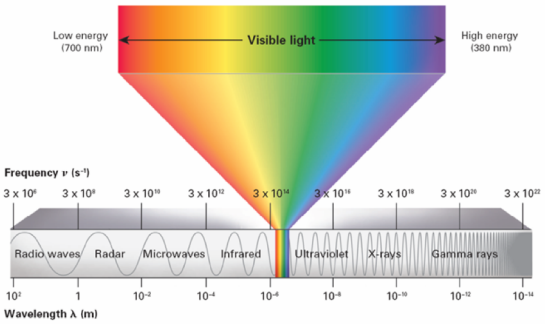
Electromagnetic Spectrum

LOW Energy — HIGH Energy

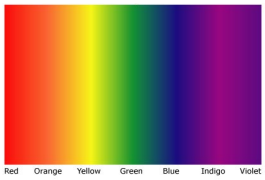
Radio	Micro-waves	Infrared	Ultra-violet	X-Rays	Gamma Rays
Low Frequency					High Frequency
Long Wavelength					Short Wavelength

Visible Light

Electromagnetic Spectrum



Visible Spectrum



- We are only able to see a very limited portion of the electromagnetic spectrum (**ROY G BIV**)
- Visible light is an example of a **continuous spectrum** (no lines or bands)
- Ranges from **red** (long λ) to **violet** (short λ)

Problems

- **EXAMPLES:**

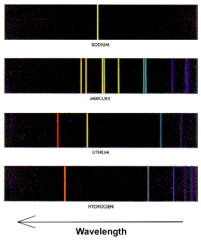
What is the **wavelength** of radiation with a frequency of 1.5×10^{13} Hz?

What is the **frequency** of radiation with a wavelength of 50.0 nm?

Atomic Emission Spectrum

Only contains certain colors or wavelengths

- Gives a pattern of color that is **UNIQUE** for each element
- Adding energy **EXCITES** an atom's electrons… so they jump from the **GROUND STATE** (lowest energy) to an **EXCITED STATE** (higher energy)
- When electrons move from a higher energy level back to a lower one, a quantum of energy (**LIGHT**) is given off that has a frequency **proportional** to the energy change…



Energy

- Energy absorbed or emitted by an atom can be calculated using: $E = h\nu$

E = **amount of energy** (J/photon)

h = **Planck's constant** = 6.63×10^{-34} J·s

ν = **frequency** of light wave

***To calculate for 1 mole, there are 6.02×10^{23} photons / 1 mol!**

- Using the $c = \lambda \nu$ equation and substitution, we know that: $E = hc/\lambda$

E is a QUANTUM of energy… like a "packet" of energy!

Problems

- **EXAMPLES:**

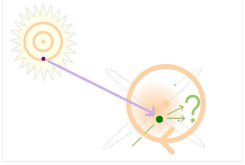
What is the **energy** in kJ/mol of 1.00 mol of photons of blue light with a wavelength of 3.60×10^{-8} m?

What is the **frequency** of the photon from above?

Heisenberg's Uncertainty Principle

Impossible to know exactly both the velocity and the position of a particle at the same time

- Does NOT apply to large objects (trains, cars, etc.) but critical in finding the position of electrons due to their small masses



Heisenberg's Uncertainty Principle

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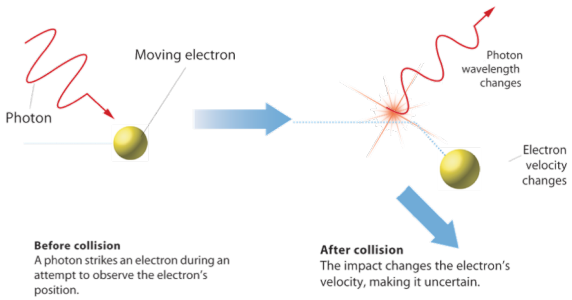
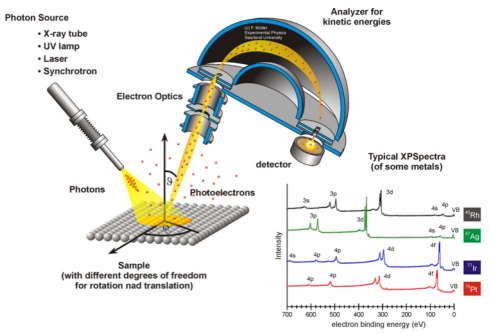


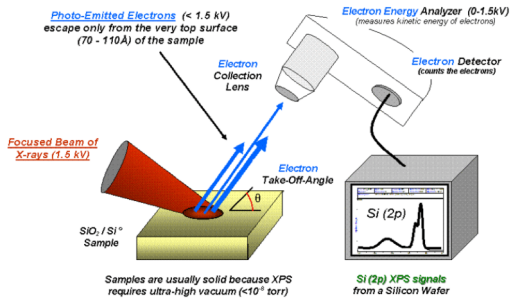
Photoelectron Spectroscopy (PES)

- Technique used to provide evidence of **ELECTRON SHELLS** in atoms (1s, 2s, etc.)
- Light is directed onto atoms and used to eject electrons (**Photoelectric Effect**)… Energy applied can be calculated using E=hv
- Electrons **CLOSER** to the nucleus (more attraction for nucleus… penetrate more) will take **MORE** energy to eject them… **MORE** energy means **GREATER** nuclear charge!!
- Peaks correspond to electrons in **DIFFERENT SUBSHELLS** and heights show the # of electrons

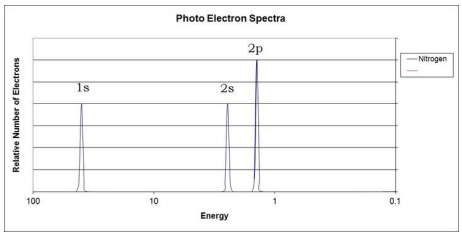
Photoelectron Spectroscopy (PES)



Photoelectron Spectroscopy (PES)

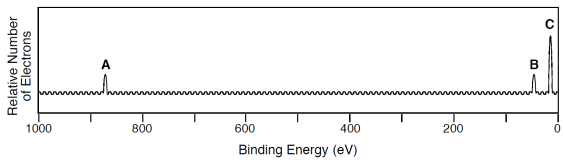


Photoelectron Spectroscopy (PES)



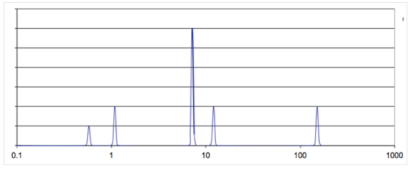
Nitrogen: $1s^2\ 2s^2\ 2p^3$

Photoelectron Spectroscopy (PES)



What do the peaks A, B, and C represent for Neon?

Photoelectron Spectroscopy (PES)



What do each of the peaks represent?

What is the identity of this element?

Beer's Law

- Used to assess the concentration of a COLORED solution by relating the absorbance of the solution to the concentration
- Graphs of absorbance vs. concentration are LINEAR

A = abc

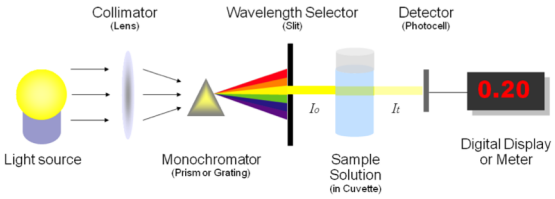
A = absorbance

a = absorptivity coefficient

b = path length (distance through solution)

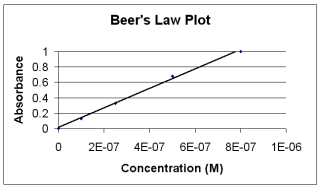
c = concentration

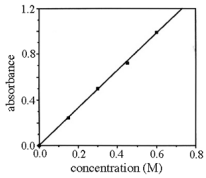
Beer's Law



The GREATER the concentration of the solution (darker it will be)… the GREATER the absorbance and the LOWER the transmittance!

Beer's Law





By using a spectrophotometer to determine the absorbance, the concentration of a colored solution can be determined using the graph / best-fit line equation / math

Beer's Law

- **EXAMPLE:**

The following data were obtained for a colored solution of a particular chemical through a 1.00 cm tube.

Concentration (M)	Absorbance
0.500	0.690
0.400	0.550
0.300	0.410
0.200	0.270
0.000	0.000

What is the absorptivity coefficient (include correct units)?

Beer's Law

- **EXAMPLE:**

The following data were obtained for a colored solution of a particular chemical through a 1.00 cm tube.

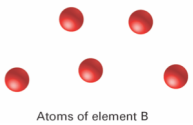
Concentration (M)	Absorbance
0.500	0.690
0.400	0.550
0.300	0.410
0.200	0.270
0.000	0.000

What is the concentration of the solution when the absorbance is 0.600?

Dalton's Atomic Theory

1) ALL elements are made of tiny, indivisible atoms

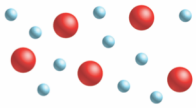
Atoms of element A



Atoms of element B

2) Atoms of the SAME element are IDENTICAL… atoms of DIFFERENT elements are DIFFERENT

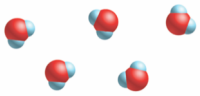
Dalton's Atomic Theory



Mixture of atoms of elements A and B

3) Atoms can mix together or combine chemically in simple whole number ratios to form **COMPOUNDS**

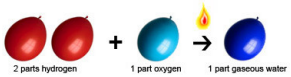
4) Chemical reactions occur when atoms are separated, joined, or rearranged… but atoms are **NEVER** changed into atoms of another element as a result



Compound made by chemically combining atoms of elements A and B

Law of Definite Proportions

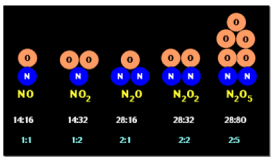
A compound always has the same elements in exactly the same proportion by mass



- Proposed by Joseph Proust
- Known as the **Law of Constant Composition**
- Ex: H_2O or H_2O_2

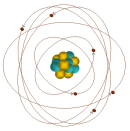
Law of Multiple Proportions

When two elements form a compound, the ratio of the masses can be reduced to whole numbers (subscripts)

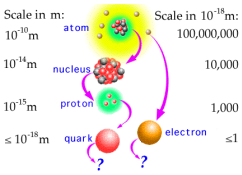


- Proposed by John Dalton
- Ex: NO (14:16 = 1:1), NO_2 (14:32 = 1:2)

Subatomic Particles

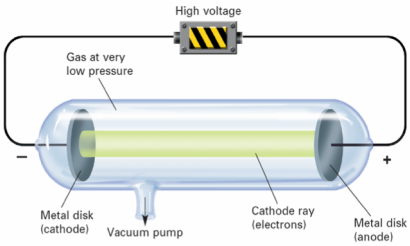


- Dalton was proved mostly right except… **ATOMS ARE DIVISIBLE**!
- Three Subatomic Particles
  - **PROTONS**: positive charge
  - **NEUTRONS**: no charge
  - **ELECTRONS**: negative charge

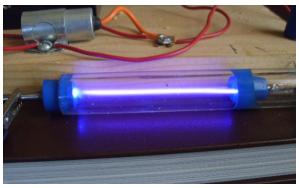


Electrons

- Discovered by **J.J. THOMSON** in 1897
- Passed a current through gases at low pressure in a vacuum tube, producing a glowing beam or **CATHODE RAY**

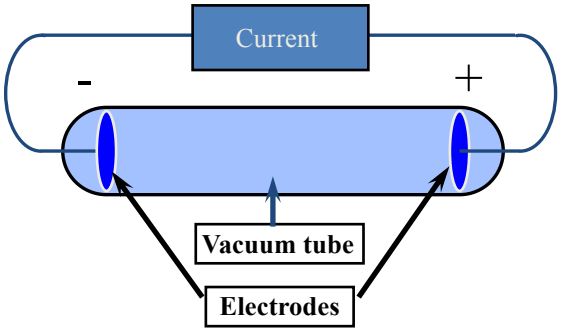


Cathode Rays

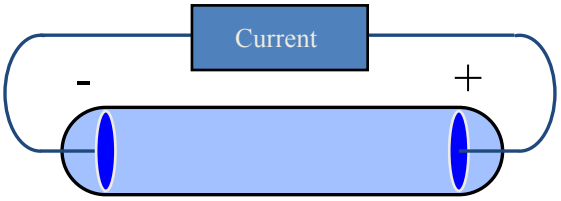


- Originate at the **NEGATIVE** end of the electrode
- Act the same regardless of the material used
- Deflected by negative magnetic fields

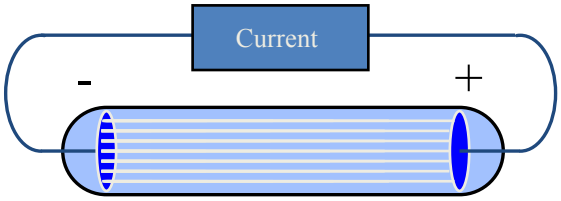
Cathode Ray Experiment



Cathode Ray Experiment

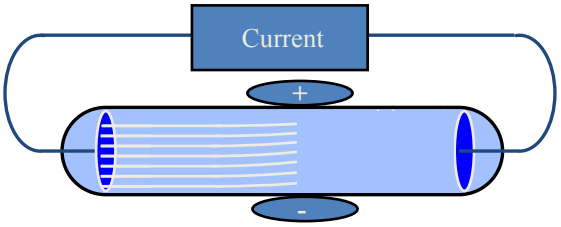


Cathode Ray Experiment



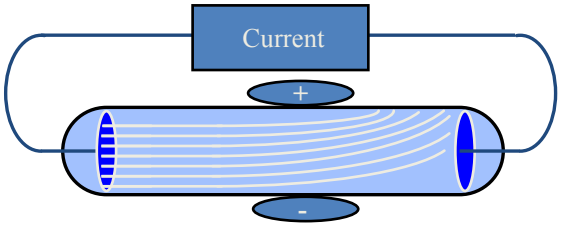
The ray is a beam of ELECTRONS traveling from the cathode to the anode!

Cathode Ray Experiment



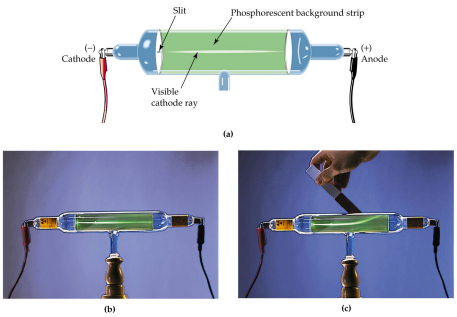
When the NEGATIVE end of a magnet is applied, the beam is repelled… ELECTRONS MUST BE NEGATIVELY CHARGED!!

Cathode Ray Experiment



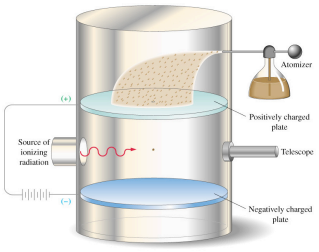
No matter what gas or metals were used, the charge-to-mass ratio remained the same… ELECTRONS ARE PART OF ALL ATOMS!!

Cathode Ray Experiment



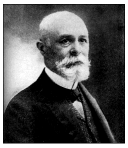
Oil Drop Experiment

- **ROBERT MILIKAN** calculated the charge and mass of the electron
- **Charge**: one unit of negative charge (-1)
- **Mass**: 1/1840 the mass of a hydrogen atom (**LIGHTEST SUBATOMIC PARTICLE**)



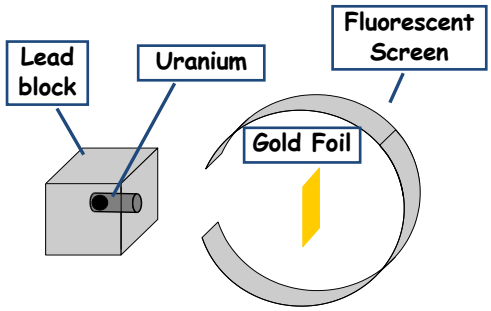
Protons and Neutrons

- **EUGENE GOLDSTEIN** discovered protons (1,840 times larger than an electron)
- **JAMES CHADWICK** confirmed the existence of neutrons (about the same size as a proton)

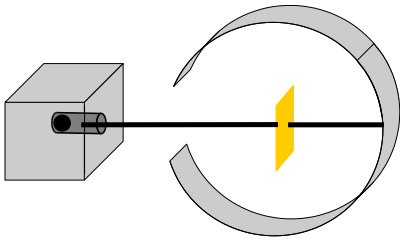


Gold Foil Experiment

- **ERNEST RUTHERFORD** shot alpha particles (positively charged) at a thin sheet of gold foil

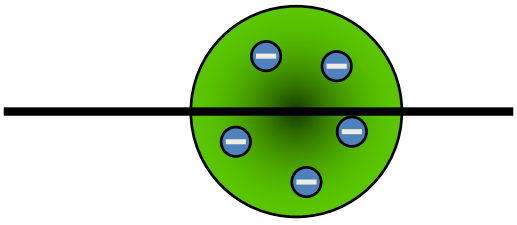


Gold Foil Experiment



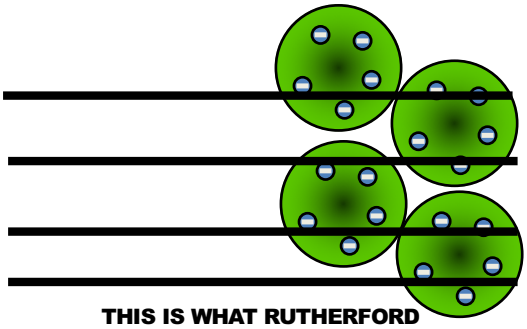
Hypothesis: alpha particles will pass through the foil WITHOUT changing direction because negatively charged particles spread out in the atoms of the foil will not stop or deflect the alpha particles

Gold Foil Experiment



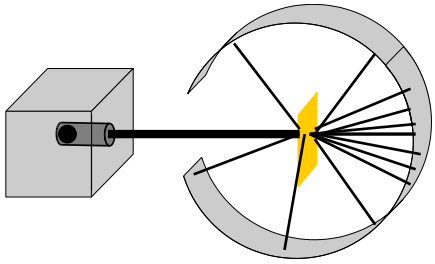
THIS IS WHAT RUTHERFORD EXPECTED!!

Gold Foil Experiment



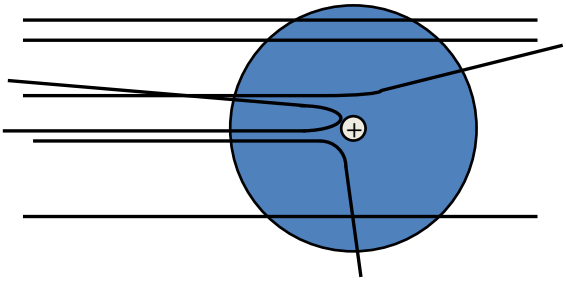
THIS IS WHAT RUTHERFORD EXPECTED!!

Gold Foil Experiment



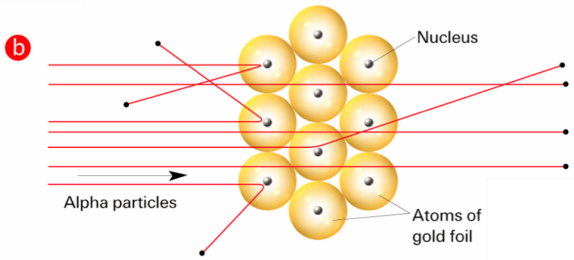
Results: most went straight through, some curved, and some came straight back

Gold Foil Experiment

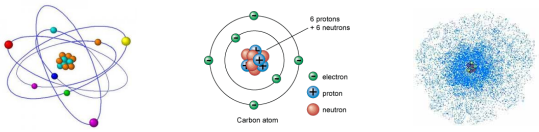


Conclusions: most of the atom is EMPTY SPACE with a dense, positively charged NUCLEUS (protons and neutrons)!!!

Gold Foil Experiment



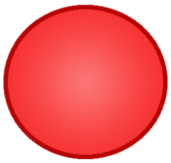
Models of the Atom



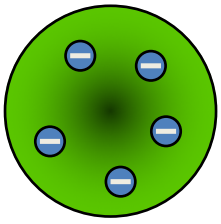
- Various scientists contributed to our understanding of the atom
- Discoveries made between 1800s – 1930s shaped the current model

Dalton's Model

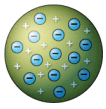
- **1803**: Views atoms as tiny and indestructible particles with **NO** internal structure



Thomson's Model



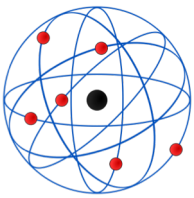
- **1897**: Negatively charged particles (electrons) are distributed throughout a uniform positive charge

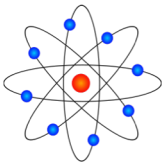


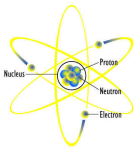
"PLUM-PUDDING" MODEL

Rutherford's Model

• **1911**: Small, dense, positively charged nucleus with the electrons moving around the nucleus (mostly empty space)

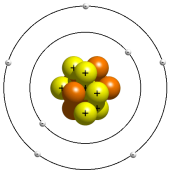




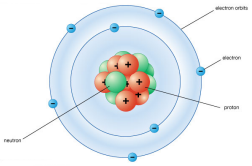


Did NOT explain the chemical properties of elements!!

Bohr's Model



• **1913**: Electrons move in a circular orbit at FIXED distances from the nucleus (NIELS BOHR)



Bohr's Model

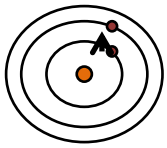
• ENERGY LEVELS (n): fixed energies an electron can have (orbits)

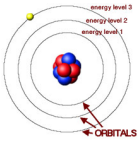
• Positive nucleus "attracts" the electrons so they stay in orbit

• Electrons absorb or emit energy as they move between levels:

-To an EXCITED (higher) orbit = ABSORBS energy

-Return to GROUND (lower) orbit = EMITS energy





Bohr's Model

• Imagine the fixed energy levels are like the RUNGS OF A LADDER: lowest rung is lowest in energy, can move rung to rung, you can't stand between the rungs just like electrons can't be in between levels, and to climb you need the right amount of energy

• Levels are **NOT** equally spaced apart, so electrons gain or lose different amounts of energy

Bohr's Model

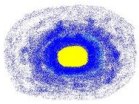
• Higher energy levels are CLOSER together… it takes LESS energy to move from one to the next near the top!

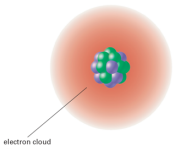
Ladder with UNEQUALLY spaced rungs is actually a better representation of the model!!

Schrodinger's Model

• **1926**: Development of a mathematical equation to determine locations around the nucleus that would have a high probability of containing an electron (ERWIN SCHRODINGER)

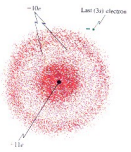
"ELECTRON CLOUD" or QUANTUM MECHANICAL MODEL (current)





Schrodinger's Model

- Protons and neutrons found in the nucleus
- ELECTRON CLOUD: visual representation of probable locations of electrons in the atom



DENSER regions = HIGHER probability of finding an electron

Distinguishing Among Atoms

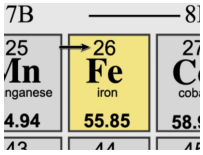
Why are atoms of different elements different?

- They contain different number of PROTONS
- PROTONS tell you which element is which!

Atomic Number (*Z*)

Number of Protons

- Use the Periodic Table to determine
- Ex: all Hydrogen atoms have one proton, so the atomic # of hydrogen is 1
- What is the Atomic Number for each: Li, Pb, Au, Br?



Electrons

Since atoms are electrically neutral, the # of protons must EQUAL the # of electrons!!

- Atoms with DIFFERENT numbers of protons and electrons are IONS (charged particles)
- Only the ELECTRONS can increase or decrease to give ions, NOT the protons… WHY?
- Positive (+) charge = LOSE electrons, while Negative (-) charge = GAIN electrons… number of charge indicates how many!

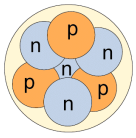
Mass Number

Sum of all the protons and neutrons in an atom (not on the Periodic Table- ROUND to get most common isotope Mass #)

MASS # = # of PROTONS + # of NEUTRONS

# of NEUTRONS = MASS # - # of PROTONS

- Example: If an element has an atomic number of 34 and a mass number of 78 what is the…
  - Number of protons?
  - Number of neutrons?
  - Number of electrons?
  - Symbol for this element?



Atomic Symbols

Mass Number

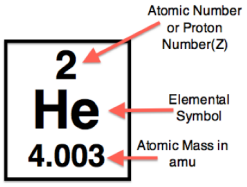
X

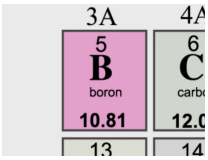
Atomic Number

- Example: If an element has 91 protons and 140 neutrons what is the…
  - Atomic number?
  - Mass number?
  - Number of electrons?
  - Atomic Symbol for this element?

Reading the Periodic Table

Round the ATOMIC MASS to get the MASS # of the most common isotope!!!



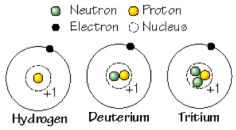


Isotopes

Atoms of the same element that have different number of neutrons

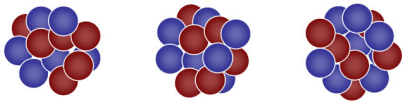
- Mass # is different because there are more or less neutrons
- Atomic # is still the SAME… otherwise the element would change!
- Naming: put the Mass # after the element name

Ex: Carbon-12, Carbon-14, Uranium-235



Isotopes

Atoms of the same element that have different number of neutrons



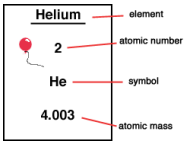
carbon-12	carbon-13	carbon-14
98.9%	1.1%	<0.1%
6 protons	6 protons	6 protons
6 neutrons	7 neutrons	8 neutrons

- **EXAMPLE:**

Determine the number of each subatomic particle for Neon-22.

Atomic Mass

Weighted average mass of the atoms in a naturally occurring sample of the element



- Reflects both the MASS and relative ABUNDANCE of the isotopes as they occur in nature
- NOT a whole number because it is an average
- Given on the Periodic Table
- Measured in Atomic Mass Units (**amu**)… 1 amu = 1/12 the mass of a Carbon-12 atom

Calculating Avg. Atomic Mass

$$\text{AVERAGE ATOMIC MASS} = \sum \left(\frac{\text{\% NATURAL ABUNDANCE}}{100\%} \right) \times \text{ISOTOPIC MASS (amu)}$$

- **EXAMPLE:**

Calculate the average atomic mass of copper if copper has two isotopes. 69.1% of copper has a mass of 62 amu and 30.9% has a mass of 64 amu.

69.1% / 100% = 0.691 **30.9% / 100% = 0.309**

0.691 X 62 amu = 42.842 **0.309 X 64 amu = 19.776**

42.842 + 19.776 = 62.618 amu

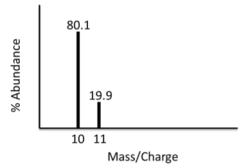
Calculating Avg. Atomic Mass

- **EXAMPLE:**

The element Gallium has two stable isotopes, Ga-69 and Ga-71. The average atomic mass of Gallium is 69.7978 amu. Find the percent abundance of each isotope of the element.

Mass Spectrometry

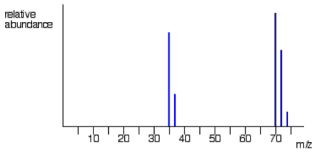
- Technique used to identify the masses of the isotopes in a naturally occurring sample of the element and find the average atomic mass
- **Mass spectrometer** (machine) produces the **mass spectra** (picture) for an element

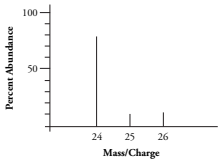


What would be the average atomic mass for this element?

Mass Spectrometry

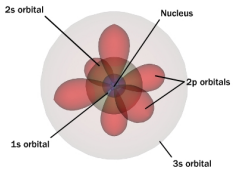
Chlorine would look like this because of Cl^- ions and Cl_2 molecules!





What element would this mass spec graph correspond to?

Quantum Mechanics



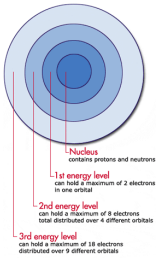
- There are **FOUR** quantum numbers that represent the address of an electron (n, l, m_l, and m_s)
- The first three describe an orbital

Remember… electrons are attracted to the nucleus and repulsed by other electrons!

Principal Quantum Number (n)

Represents the energy level

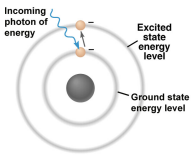
- Regions in space around the nucleus that contain electrons
- Tell you how close an electron is to the nucleus
- n = 1-7… with 1 being the **LOWEST** in energy and **CLOSEST** to the nucleus

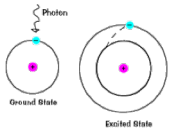


CLOSER to nucleus = LOWER in energy… but PENETRATE the nucleus more!

Principal Quantum Number (n)

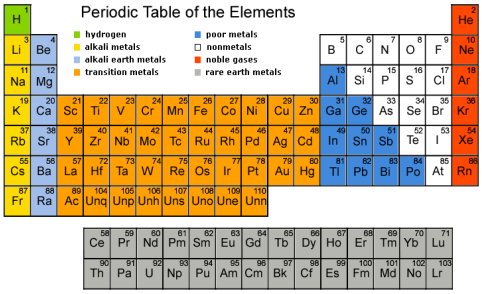
Represents the energy level





- **GROUND STATE** (lowest energy) is N = 1
- **EXCITED STATES** (higher energy) are N = 2 , N = 3, etc.
- Electrons in excited states are farther from the nucleus, have larger orbits, and more energy!
- Maximum # of e- in an energy level found using $2n^2$

Principal Quantum Number (n)

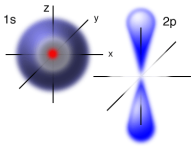


ROWS on the Periodic Table indicate the energy level!!

Azimuthal Quantum Number (l)

Represents the shape of the orbital

- Principal energy levels can be divided into energy SUBLEVELS or SUBSHELLS
- Each energy level can have several sublevels with different shapes (showing where an electron is likely to be found)
- Sublevels are denoted by letters: s, p, d, f

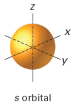


INCREASING ENERGY

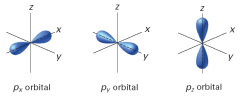
s electrons penetrate the nucleus more… ATTRACTED more so less energy!

Azimuthal Quantum Number (l)

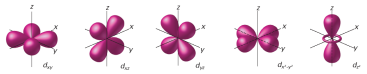
Represents the shape of the orbital



s
l = 0
2 e- Max
Spherical



p
l = 1
6 e- Max
Dumbbell

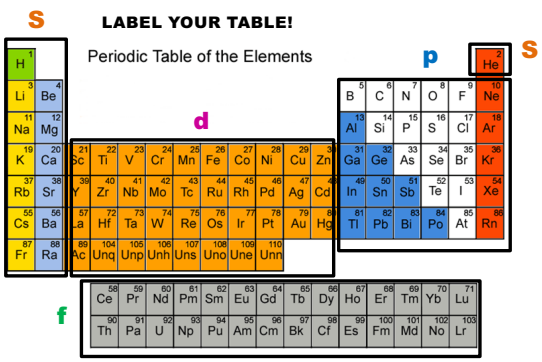


d
l = 2
10 e- Max
Double Dumbbell

f **Crazy!**
l = 3
14 e- Max

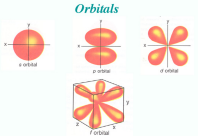
Sublevels on the Periodic Table

LABEL YOUR TABLE!



Magnetic Quantum Number (m_l)

Orientation of an orbital / Regions within a sublevel that can hold a maximum of 2 e-

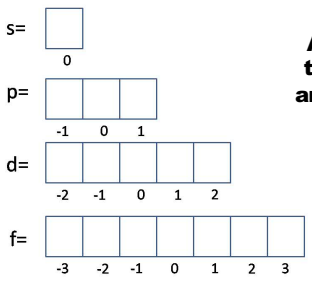


- Electrons are spinning in opposite directions… "Orbital Pair"
- Range of numbers from -3 through +3 (-/through +/including 0)
- Each sublevel has a different number of orbitals: s = 1, p = 3, d = 5, and f = 7
- Since each orbital can hold 2 e-, max # of e- determined by:

# of orbitals x 2

Magnetic Quantum Number (m_l)

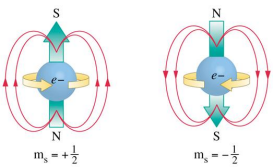
Orientation of an orbital / Regions within a sublevel that can hold a maximum of 2 e-



Always put "0" in the middle orbital and then –/through zero to +/

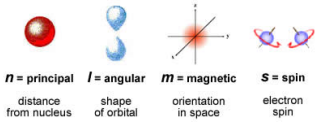
Spin (m_s)

Distinguishes between the electrons in an orbital



- Only two possible values: -1/2 or +1/2 (indicates that the electrons in the pair have OPPOSITE spins)
- Electrons are shown to have different spins when drawing the electron diagrams

Quantum Numbers



Summary

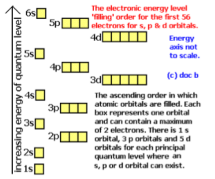
ENERGY LEVEL (n)	# OF SUBS	# OF ORBS (n^2)	MAX # OF e^- ($2n^2$)
1	1 (S)	1	2
2	2 (S & P)	4	8
3	3 (S, P & D)	9	18
4	4 (S, P, D, F)	16	32

Electron Configurations

Shows distribution of electrons among the orbitals of the atom

THREE WAYS TO DO THIS:

- Orbital Diagrams (using boxes with electrons as arrows)
- SPDF Notation (letters and numbers showing levels and electrons)
- Kernel Notation (use noble gases and simplified SPDF)



Rules

1) AUFBAU PRINCIPLE: add electrons one at a time to the orbitals of **LOWEST** energy first

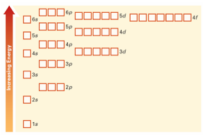
2) PAULI EXCLUSION: e- **MUST** have opposite spins and **MAX** of 2 e- per orbital (each e- has **FOUR** different quantum #s)

3) HUND'S RULE: each orbital in the sublevel must have one e- **BEFORE** pairing begins

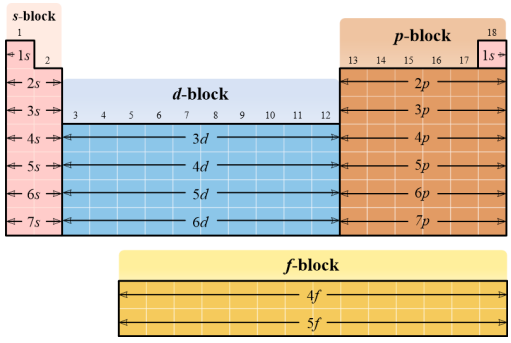
Orbital Diagrams

HOW TO DRAW:

1) Use a box to represent one orbital / Arrows represent electrons
2) Find the # of electrons
3) Start with the lowest energy level first (n = 1) and write down all sublevels in each
4) Follow all rules (max 2 e- per orbital, correct # of orbitals for spdf, unpaired first, d is one row behind)
5) Use the Periodic Table to help!



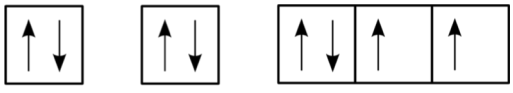
Orbital Diagrams



Assigning Quantum Numbers

- **EXAMPLE:**

Draw the orbital diagram for oxygen. Assign four **quantum numbers** to each electron.



1, 0, 0, +1/2
1, 0, 0, -1/2

2, 0, 0, +1/2
2, 0, 0, -1/2

2, 1, -1, +1/2
2, 1, -1, -1/2

2, 1, 1, +1/2

2, 1, 0, +1/2

ALL ELECTRONS HAVE A DIFFERENT ADDRESS... FOUR DIFFERENT QUANTUM #S!!

Assigning Quantum Numbers

- **EXAMPLE:**

Draw the orbital diagram for aluminum. Assign four **quantum numbers** to each electron.

Magnetic Fields

PARAMAGNETIC

Has one or more unpaired electrons... attracted to magnetic field

Ex: Hydrogen

DIAMAGNETIC

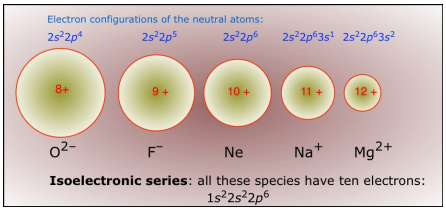
All electrons are paired... slightly repelled by magnetic field (magnetism Dies!)

Ex: Helium

Relates directly to the two spins possible (+1/2 and -1/2)... Cancel out for Diamagnetic!

Isoelectronic Species

Share the same electron configuration (usually due to charges), but have different radii



GREATER the nuclear charge... SMALLER the species!

SPDF Notation

- The electron configuration for chlorine using this notation is:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

-Large numbers represent the energy level

-Letters represent the energy sublevel

-Superscript numbers indicate the number of electrons in the sublevel

USE THE PERIODIC TABLE TO GUIDE YOU!!

Kernel (Shorthand) Notation

- Write the symbol of the noble gas (**FARTHEST RIGHT** column on the table) that PRECEDES the element on the Periodic Table and put in [ ]
- Then write the remaining electrons using spdf notation
- **EXAMPLE:**

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

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

So... Al is: **[Ne] $3s^2\ 3p^1$**

Try Ca and Sb on your own!

Exceptions

- Some electron configurations will be different than what is expected from the rules
- **WHY?…** Less electron-electron repulsions!!!!
- Examples: Chromium and Copper (one electron is moved for added stability)

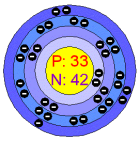
Cr: $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$ $4s^1$ $3d^5$

Try Cu on your own!

Valence Electrons

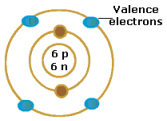
Electrons in the outermost energy level (ones involved in chemical reactions)

- Usually **HIGHEST** energy level s **AND** p electrons added together
- Ex: As



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

5 valence electrons



- More Ex: Ne, Mg, C, and Cl

Electron Dot Structures

Diagrams that show valence electrons as dots around the element symbol

(also known as "Lewis Structures")

- **How to draw:**

1)Determine the # of valence e-

2)Write the element symbol

3)Add one e- at a time to each side of the symbol… show as dots

4)Until they are forced to pair up (8 e- max)

EXAMPLE: Nitrogen