Atomic Structure

Ms. Peace

Lesson 1

The Nuclear Atom

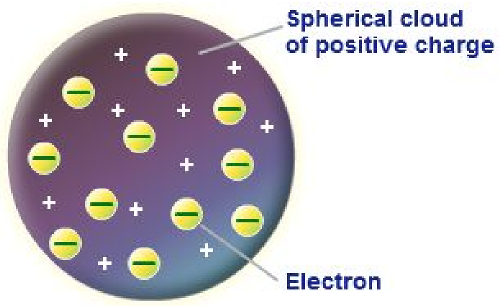
Main

Dalton's Theory

- In 1808 John Dalton developed an atomic model that was supported by experimental data
- This model formed the origin of atomic theory
- This model was refined and replaced over time
- Four postulates remain true today:
  - 1. All matter (materials) consist of very small particles called atoms
  - 2. An element consists of atoms of one type only
  - 3. Compounds consist of atom of more than one element and are formed by combining atoms in whole-number ratios
  - 4. In a chemical reaction atoms are not created or destroyed

Thomson's Model

- In 1906 Thomson won a Nobel Prize in Physics for the discovery of the electron
- Thomson proposed the "plum-pudding" model of the atom-the atom was similar to a plum pudding (a dessert eaten on Christmas day in the UK and Ireland) with negatively charged particles (the raisins) embedded in a positive region (the pudding) of the atom

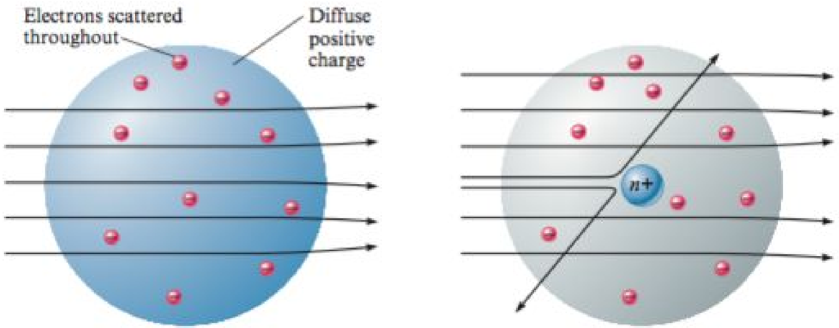


Thomson's Plum pudding model

Rutherford's Experiment

- In 1909 Rutherford and his co-workers conducted the gold foil experiment
- A thin gold metal foil was placed in an evacuated chamber and bombarded with alpha particles
- Alpha particles are high-energy positively charged He^{2+} ions
- Most of the particles went through the gold foil and some were deflected slightly and some greatly
- This led to the discovery of the

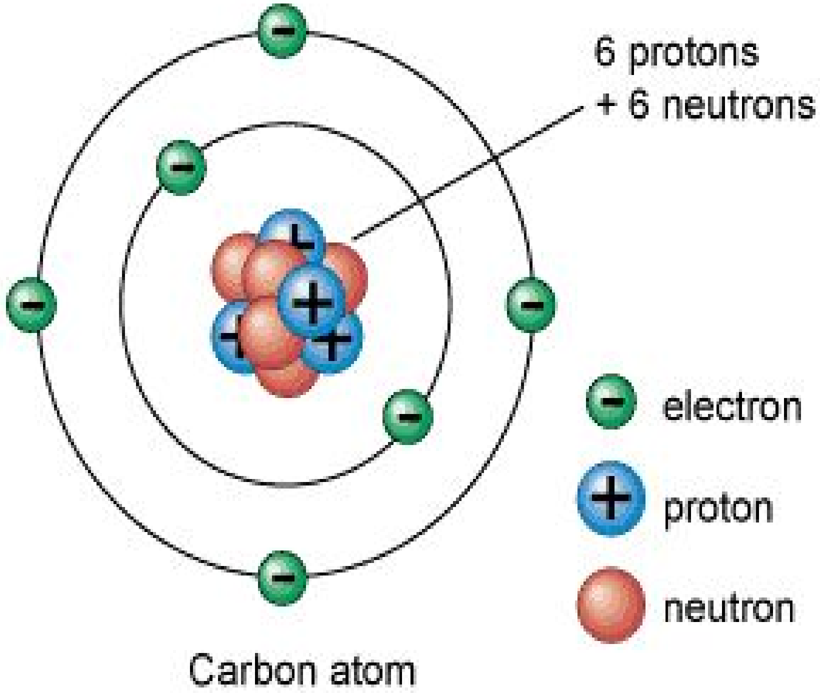
nucleus



Main

Subatomic Particles

- Atoms contain protons (+) and neutrons that are sometimes referred to as nucleons
- Electrons (-) occupy space outside of the nucleus



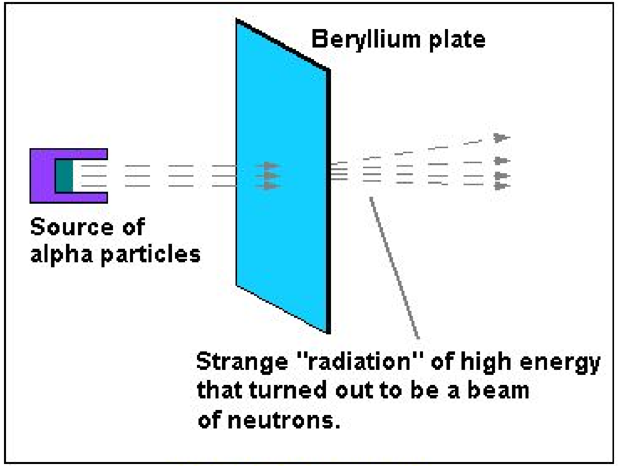
Subatomic Particles

Particle	Relative Mass	Relative Charge
Proton	1 amu	+1
Neutron	1 amu	0
Electron	1/1836 amu	-1

1 amu = 1.660539×10^{-24}g

Discovery of the Neutron

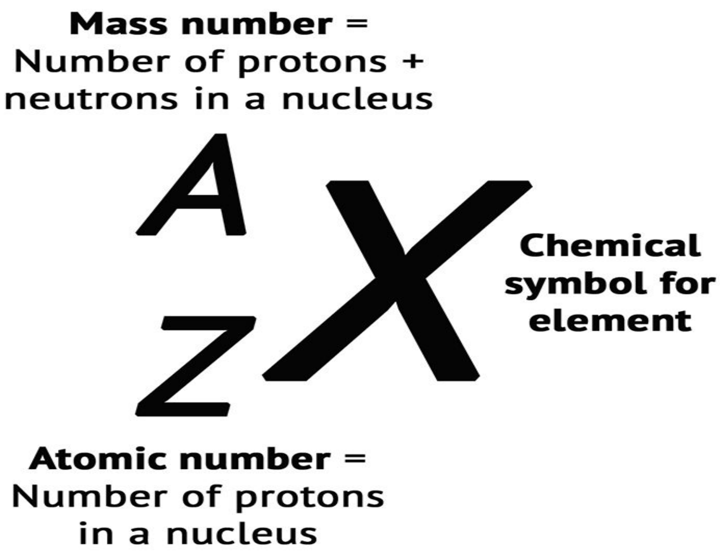
- The neutron was discovered by James Chadwick in 1932
- His discovery was based on the experiment in which Beryllium was placed in a vacuum chamber and bombarded with He^{2+} ions
- Beryllium was found to emit neutrons and he was able to prove that the particles were indeed neutrons
- Solved the last piece of the puzzle on atomic structure



Detection of neutrons

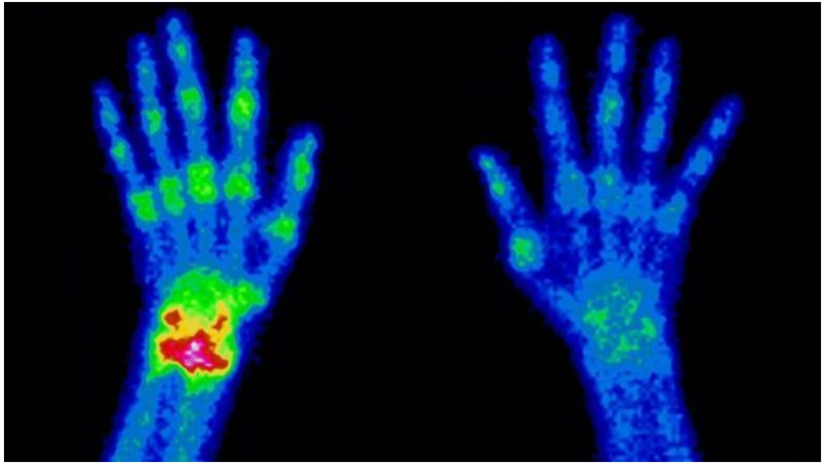
Nuclear Symbol Notation

- The atomic number, Z, is the number of protons in the nucleus of the atom of an element
- For neutral atoms, the number of electrons equals the number of protons
- The mass number, A, is the number of protons + neutrons in the nucleus



Radioisotopes

- Isotopes differ in the number of neutrons resulting in different mass numbers
- Radioactive isotopes are used in nuclear medicine for:
  - Diagnostics
  - Treatment
  - Research
  - Tracers
  - Geological clocks



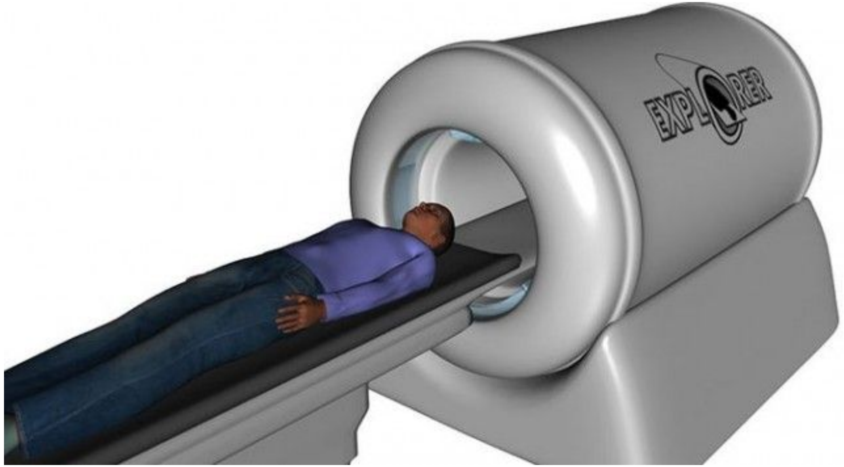
Main

Isotopes

- Different atoms of the same element with different mass number (different numbers of neutrons in the nucleus)
- Consider ^{35}Cl and ^{37}Cl, most naturally occurring samples of elements are composed of mixtures of isotopes but usually one isotope is far more abundant that the others and the mass number of the most common isotope is quoted
- Isotopes have the same chemical properties (they react in exactly the same way) but different physical properties, i.e. melting points and boiling points

PET Scans and SPECT Imaging

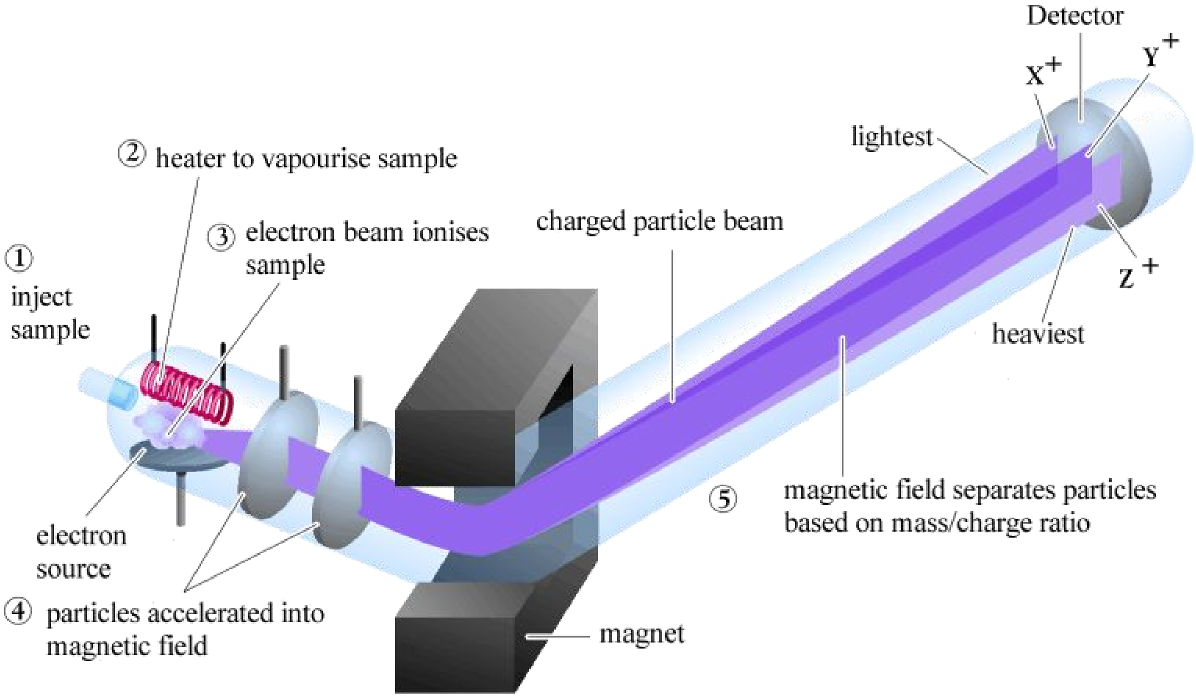
- Positron Emission Tomography (PET) scanners give 3-D images of tracers concentration in the body and can be used to detect cancers
- Single-Photon Emission Computed Tomography (SPECT) imaging can be used to detect the gamma rays emitted in iodine-131, used in the treatment of thyroid cancer and to determine which thyroid gland is functioning normally



Main

Mass Spectrometer

- An instrument used to determine the relative atomic mass of an element



Main

Operation of the Mass Spectrometer

1. ***Vaporization:*** The sample is injected into the instrument where it is heated and vaporized, producing gaseous atoms or molecules

2. ***Ionization:*** The gaseous atoms are bombarded by high-energy electrons, generating positively charged species:

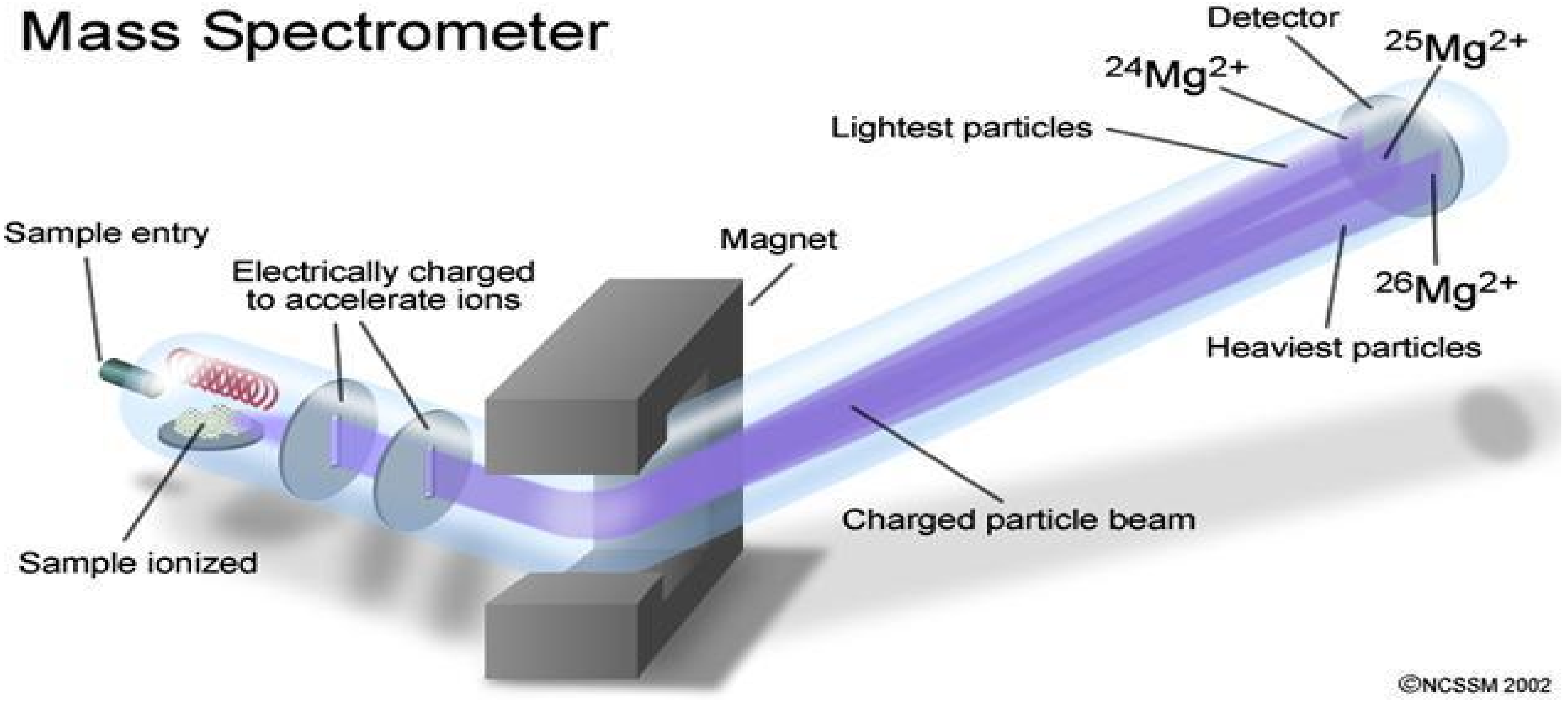
$$X(g) + e^- \rightarrow X^+(g) + 2e^-$$

3. ***Acceleration:*** The positive ions are attracted to negatively charged plates and accelerated in the electric field

Operation of the Mass Spectrometer

4. ***Deflection:*** The positive ions are deflected by a magnetic field perpendicular to their path. The degree of deflection depends on the mass-to-charge ratio (m/z). The species with the smallest mass and highest charge will be deflected the most. Particles with no charge are not deflected in the magnetic field.

5. ***Detection:*** The detector detects species of a particular m/z ratio. The ion hits the counter and electrical signal is generated.


Mass Spectrometer
Detector
25Mg2+
24Mg2+
Lightest particles
Sample entry
Magnet
Electrically charged
to accelerate ions
26Mg2+
Heaviest particles
Charged particle beam
Sample ionized
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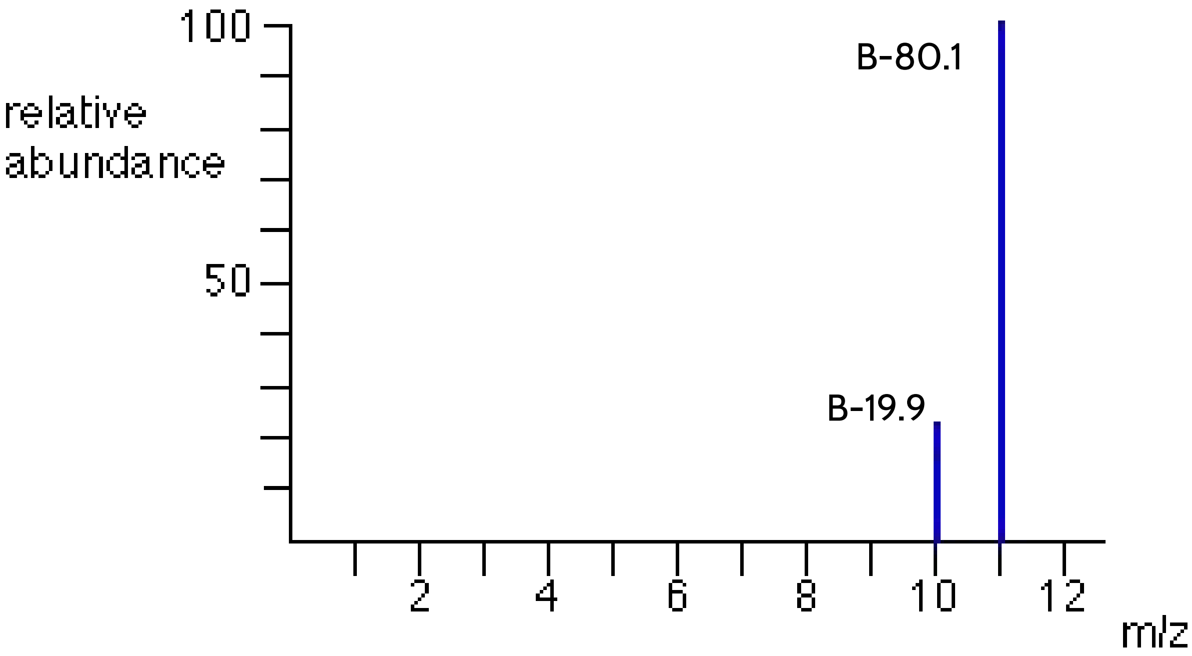
Mass Spec Graph



Each peak represents an isotope

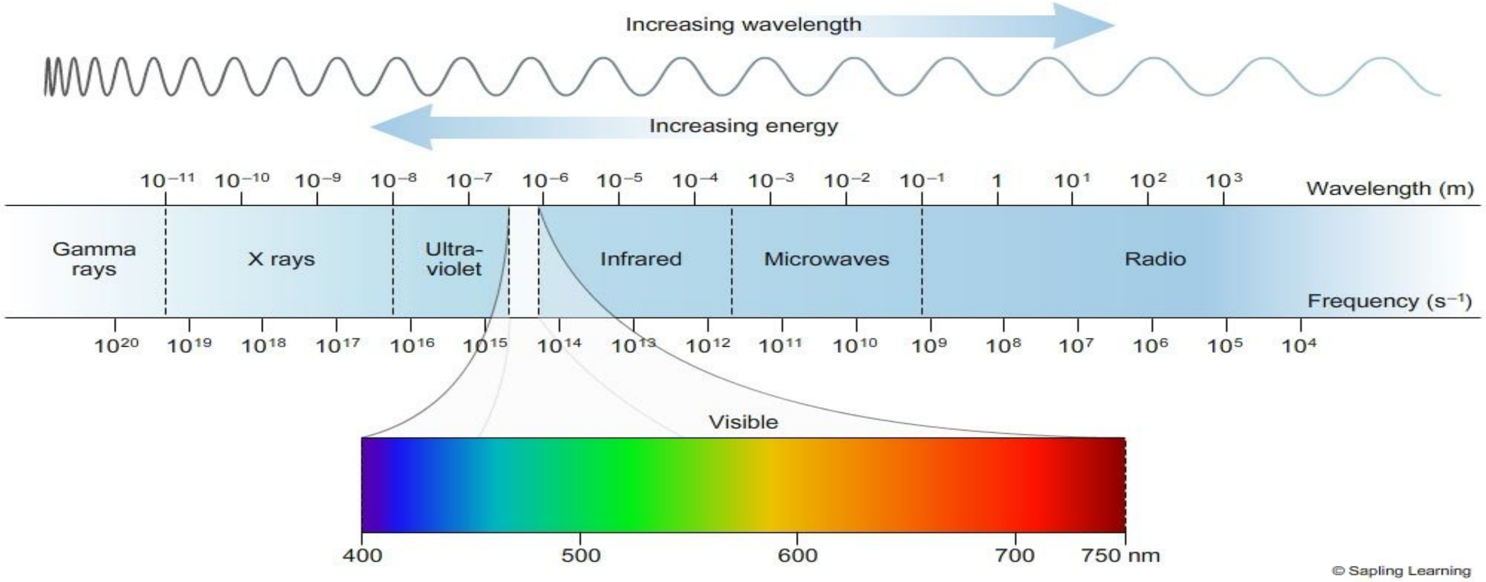
Main

Lesson 2

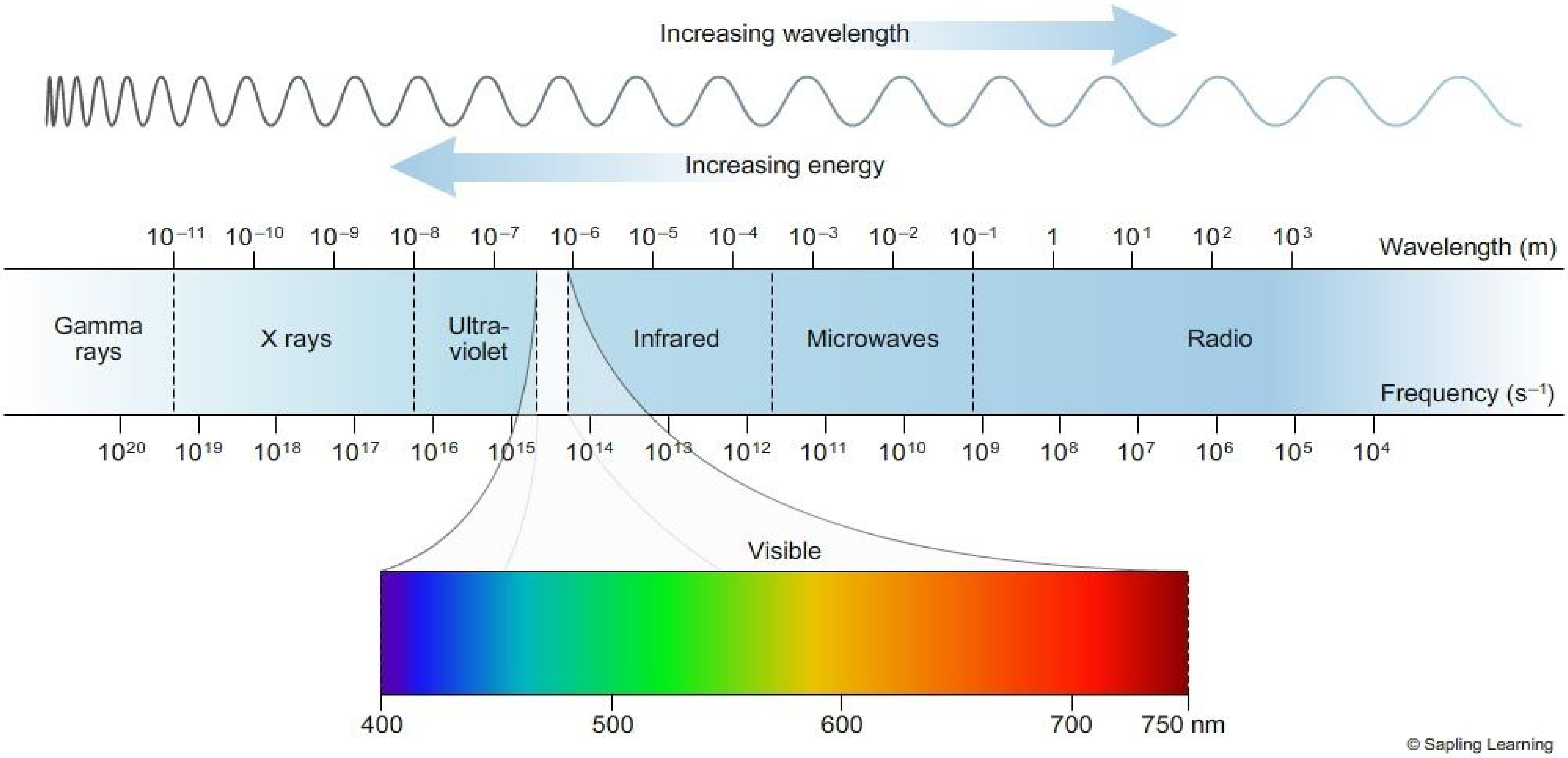
Electron Configuration Part A

The Electromagnetic Spectrum

- The electromagnetic spectrum (EMS) is a spectrum of wavelengths that comprise the various types of electromagnetic radiation



Main


Increasing wavelength
Increasing energy
10⁻¹¹ 10⁻¹⁰ 10⁻⁹ 10⁻⁸ 10⁻⁷ 10⁻⁶ 10⁻⁵ 10⁻⁴ 10⁻³ 10⁻² 10⁻¹ 1 10¹ 10² 10³
Wavelength (m)
Gamma rays
X rays
Ultra-violet
Infrared
Microwaves
Radio
Frequency (s⁻¹)
10²⁰ 10¹⁹ 10¹⁸ 10¹⁷ 10¹⁶ 10¹⁵ 10¹⁴ 10¹³ 10¹² 10¹¹ 10¹⁰ 10⁹ 10⁸ 10⁷ 10⁶ 10⁵ 10⁴
Visible
400
500
600
700
750 nm
© Sapling Learning

The Electromagnetic Spectrum

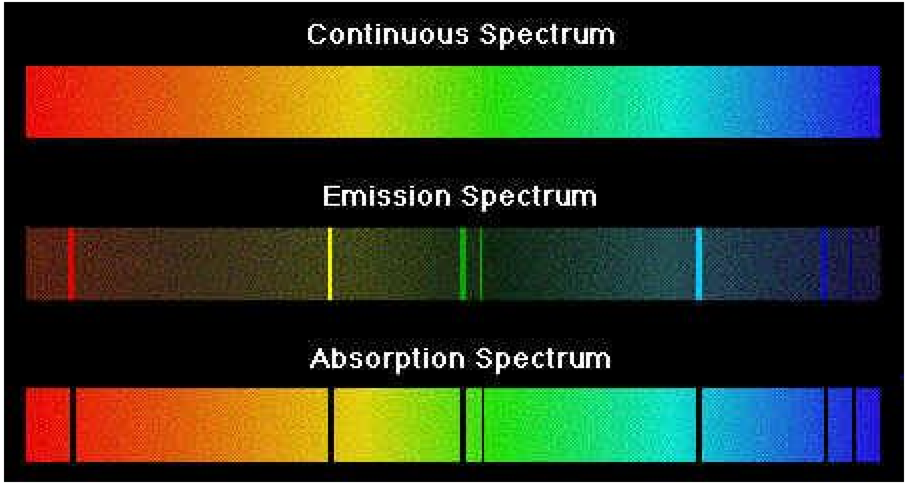
- Energy is inversely proportional to the wavelength

$$E \alpha 1/\lambda$$

- Wavelength is directly related to frequency:
  - $c = \upsilon\lambda$
  - $c = 3.00 \times 10^{8}\ ms^{-1}$
- SI units:
  - Energy: joules, J
  - Wavelength: meter, m
  - Frequency: hertz, Hz or s^{-1}

Emission Spectra

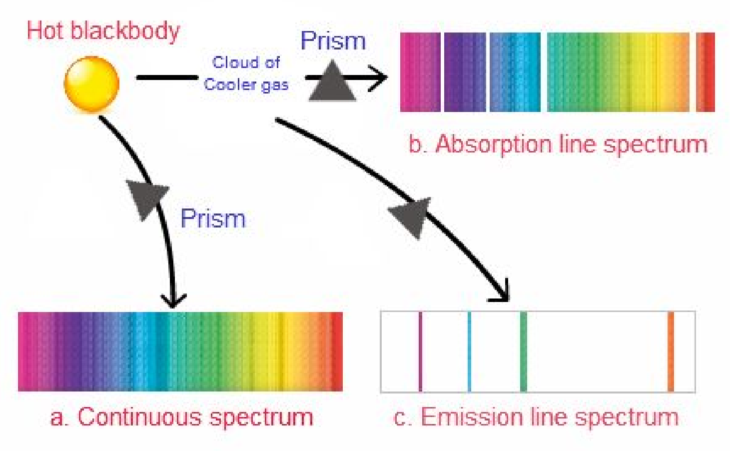
- Emission spectra are produced when photons are emitted from atoms as excited electrons return to a lower energy level.



- In the absorption spectrum, gaseous atoms absorb certain wavelengths of light from the continuous spectrum

Hydrogen Atom

- If a pure gaseous element is subjected to a high voltage under reduced pressure, the gas will emit a certain characteristic color of light
- The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies



Main

Quantization of Energy

- The precise lines in the line emission of an element have specific wavelengths
- Each characteristic wavelength corresponds to a discrete amount of energy
- Quantization is the idea that electromagnetic radiation comes in “parcels” or quanta

Quantization of Energy

- A photon is a quantum of radiation, and the wavelength and energy of a photon are related

$$E = h\nu = \frac{hc}{\lambda}$$

  - h: Plank's constant = 6.63 x 10^{-34}J s
  - ʋ: frequency of radiation
  - c: speed of light = 3.00 x 10^{8} ms^{-1}

Explanation of Spectra

- In 1913, Neils Bohr proposed a theoretical explanation for the emission spectrum of the hydrogen atom

1. The hydrogen atom consists of protons at the center, while electrons orbit in a circular path. The attraction between the two is balanced by the acceleration of the electron moving in its orbit
2. Each orbit has a definite energy associated with it. The energy in a particular orbit is fixed or quantized

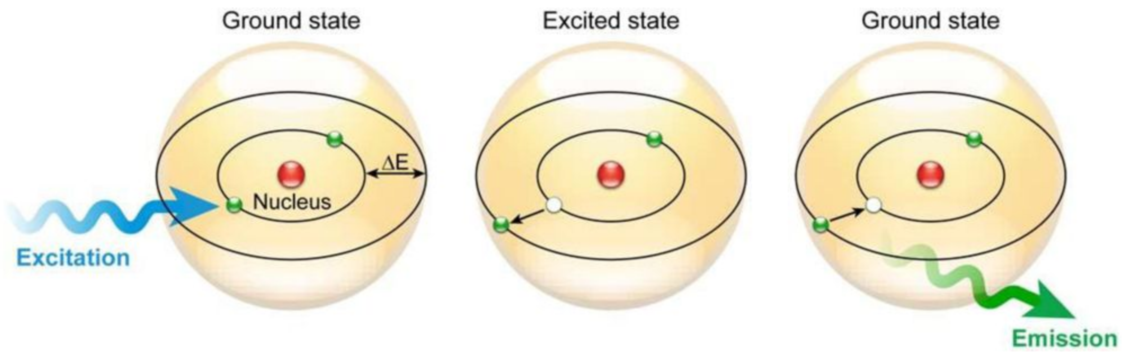
   $E = -R_n(1/n^2)$

   R: Rydberg constant = 2.18×10^{-18}J

   n: principle quantum number' positive integers

Electron States

- When an electron in its ground-state is excited, it moves to a higher energy level and stays in the excited-state for a fraction of a second
- When the electron falls back down from the excited-state to a lower energy level it emits a photon, a discrete amount of energy, which corresponds to a particular wavelength



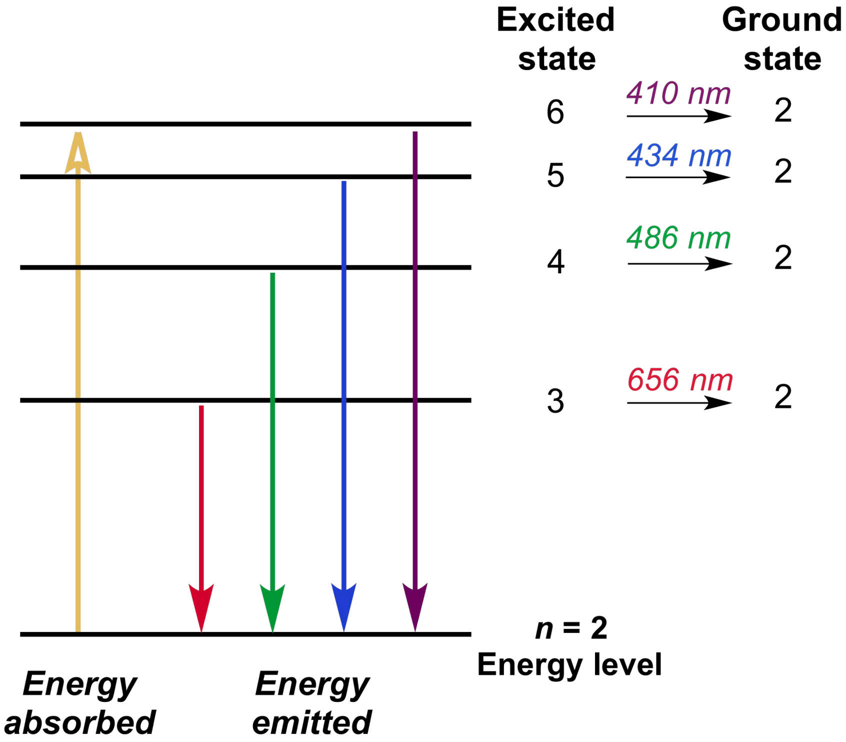
Electron States

- An electron can be excited to **any** energy level higher than its current level
- The electron can also fall back down to any lower energy level

$$\Delta E = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

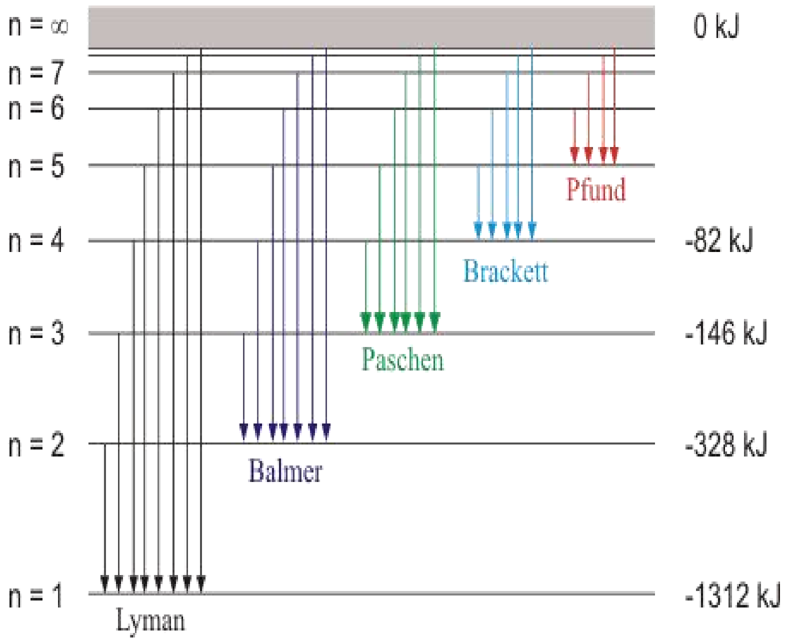
Hydrogen Atom

- The Balmer series comprises lines associated with electronic transitions from upper energy levels back down to the n=2 energy level



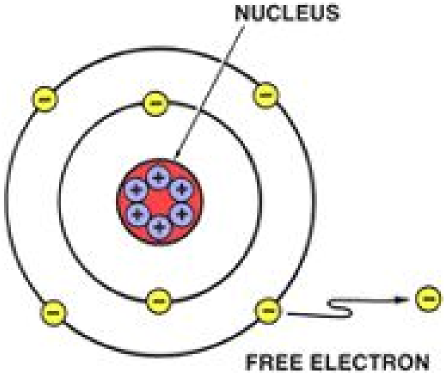
Line Series

Series	n_f	n_i	Region of EMS
Lyman	1	2,3,4,5…	UV
Balmer	2	3,4,5,6…	Visible and UV
Paschen	3	4,5,6,7,…	IR



Quantization and Atomic Structure

- The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which get closer together (converge) at higher energy levels
- At the limit of this convergence the lines merge, forming a continuum
- Beyond this continuum electrons can have any energy; it is no longer under the influence of the nucleus and is outside of the atom; called a free electron



Lesson 3

Electron Configuration Part B

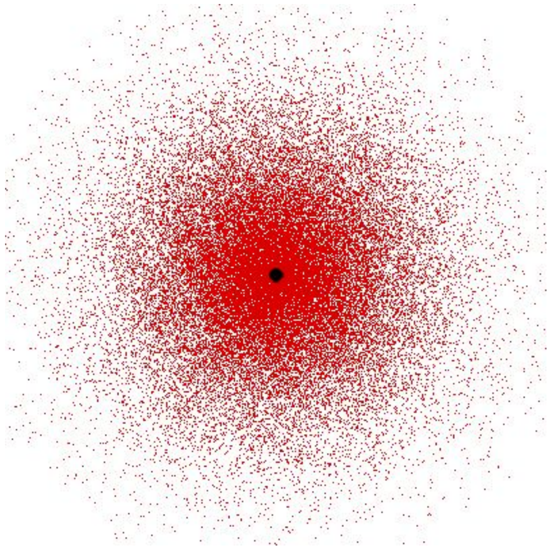
Main

Electron Arrangement

- Electron arrangements are useful for explaining and predicting the chemical properties of an element
- Heisenberg's uncertainty principle allows us to calculate the probability of finding an electron in a given region of space within the atom
- Schrödinger's equation describe possible energy states the electron can occupy
- An atomic orbital is a region in space where there is a high probability of finding an electron

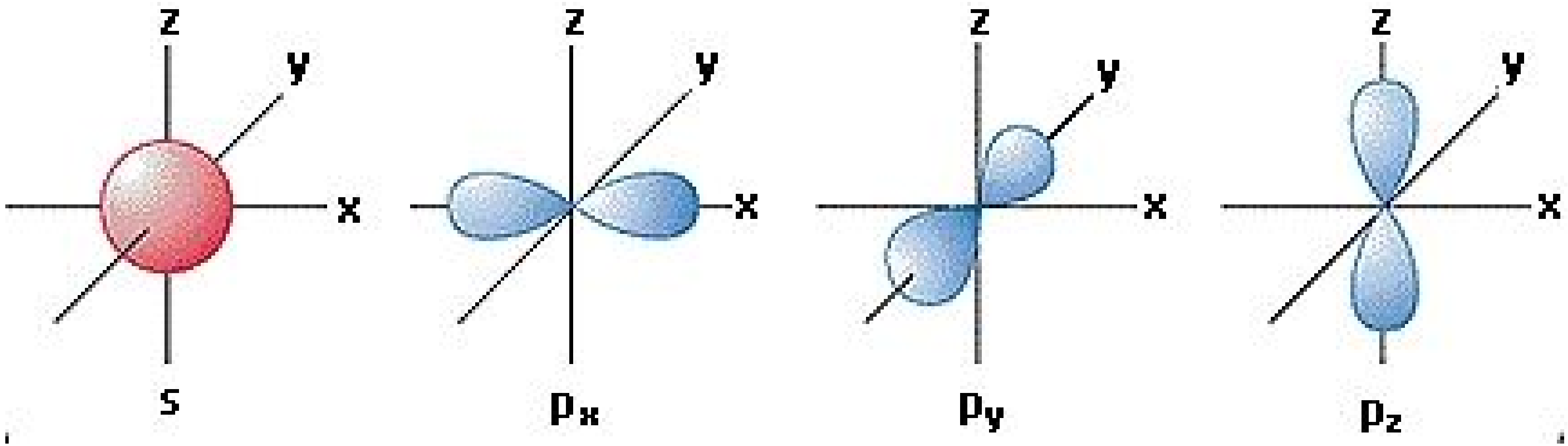
Atomic Orbital

- Any orbital can hold up to two electrons
- Each atomic orbital, s, p, d, f, have characteristic shapes and associated energies



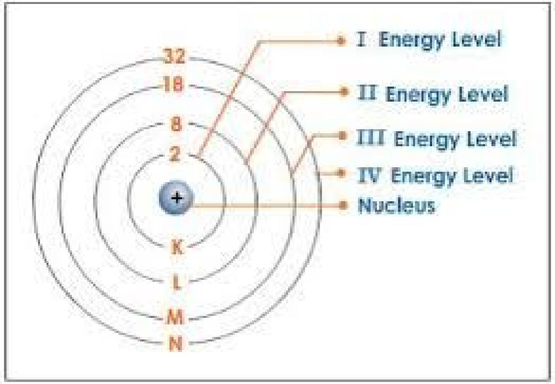
Atomic Orbitals

- S-orbital: spherically symmetrical
- P-orbital: dumbbell shaped



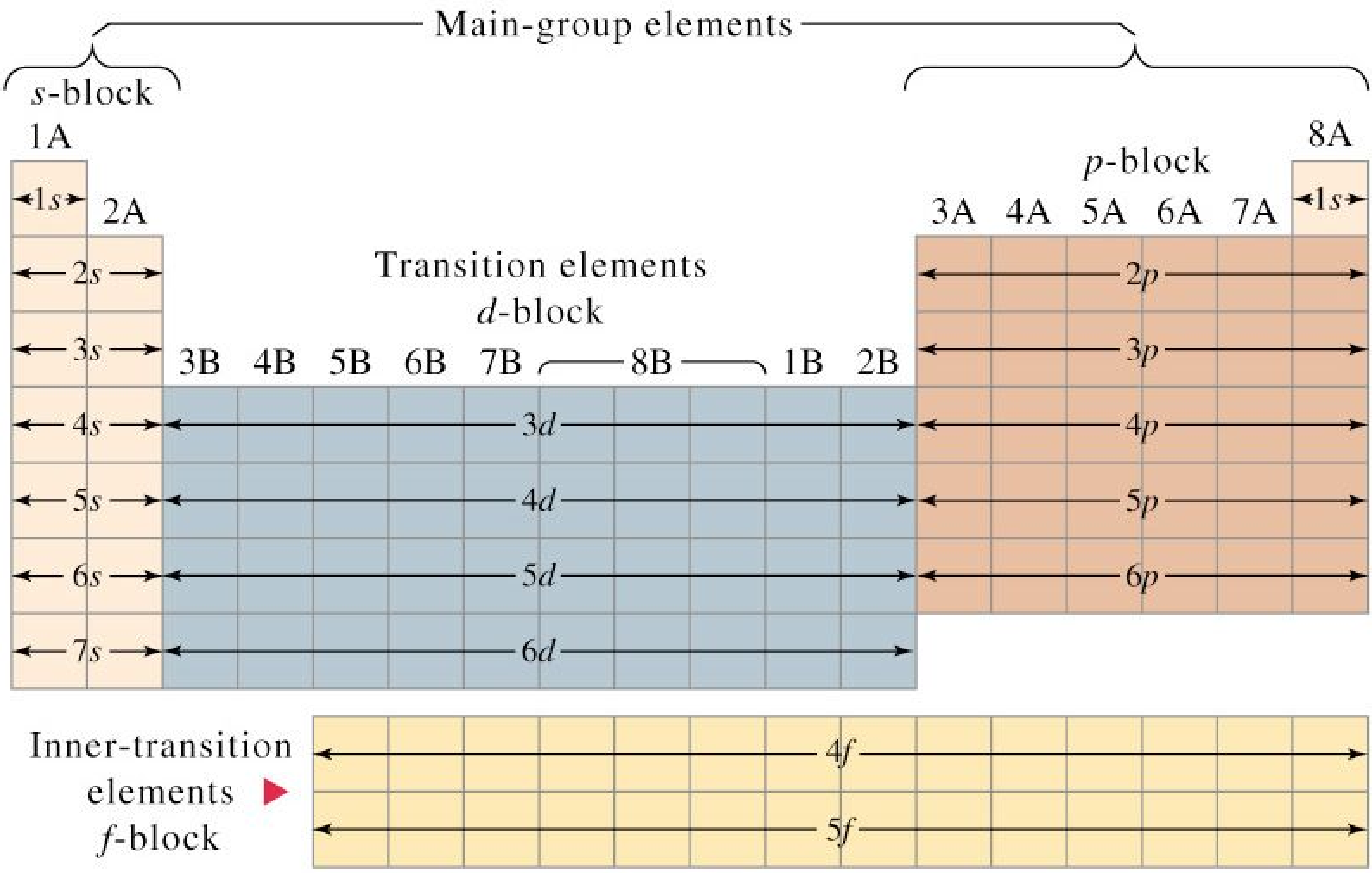
Energy Levels

- Main energy levels, principle quantum numbers, n, are positive integer values such as 1, 2, 3, 4…
- Energy levels increase as n increases
- Each main energy level or shell can hold a maximum number of electrons by $2n^2$



Sublevels

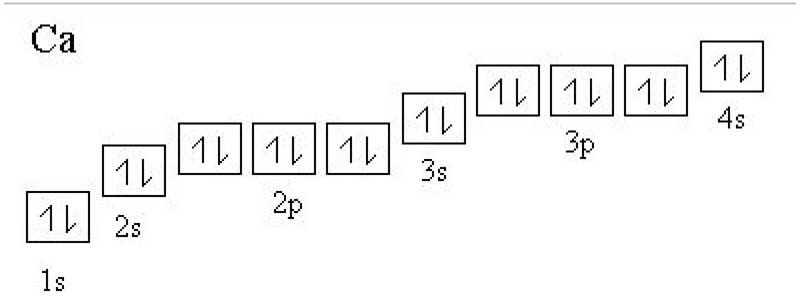
Sublevel	Number of orbitals in sublevel	Maximum Number of Electrons in Sublevel
s	1	2
p	3	6
d	5	10
f	7	14



Main-group elements
s-block
1A
1s
2A
p-block
8A
3A 4A 5A 6A 7A
Transition elements
d-block
3B 4B 5B 6B 7B 8B 1B 2B
2s
3s
4s
5s
6s
7s
2p
3p
4p
5p
6p
3d
4d
5d
6d
Inner-transition elements
f-block
4f
5f

Orbital Diagrams

- Arrows represent electrons and boxes represent orbitals



- Two electrons in the same orbital must have opposite spins
- Electrons behave as magnets facing in opposite directions

Quantum Numbers

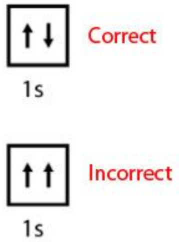
Quantum number	Name	What it labels	Possible values	Notes
n	principal	electron energy level or shell number	1, 2, 3, ...	Except for d-orbitals, the shell number matches the row of the periodic table.
ℓ	azimuthal	orbital type: s, p, d, f	0, 1, 2, ..., n-1	0 = s orbital 1 = p orbital 2 = d orbital 3 = f orbital
m_ℓ	magnetic	orbital sub-type	integers between and including $-\ell$ and $+\ell$: $-\ell, -\ell+1, \ldots \ell-1, \ell$	$\ell = 0$ (s): 2 e^- in one orbital $\ell = 1$ (p): 2 e^- in each of three sub orbitals (p_x, p_y, p_z) $\ell = 2$ (d): 2 e^- in each of 5 sub orbitals (d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$, d_{z^2})
m_s	spin	electron spin	$\pm\frac{1}{2}$	Spins in any single sub-orbital must be paired.

*Up arrow = +½, down arrow = −½

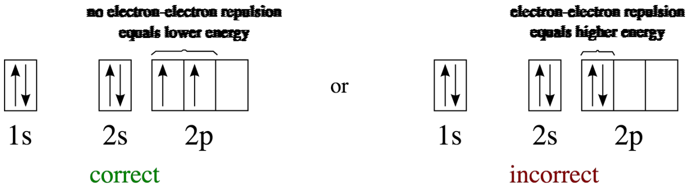
Main

Electron Configurations

1. Aufbau Principle: electrons fill the lowest-energy orbital that is available
2. Pauli Exclusion Principle: any orbital can hold a maximum of two electrons with opposite spins



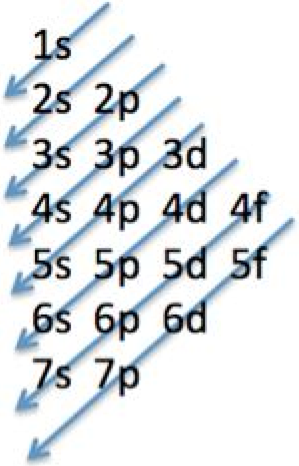
3. Hund's Rule: when filling degenerate (of equal energy) orbitals, electrons fill all the orbitals singly before occupying them in pairs



Main

Electron Configurations

- Full electron configuration



$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$
$3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2$
$4f^{14}\ 5d^{10}\ 6p^6\ 7s^2\ 5f^{14}\ 6d^{10}\ 7p^6$

Diagonal Rule

Electron Configurations

- Condensed electron configuration: convenient way of representing valence electrons

[Nearest Noble Gas] valence electrons

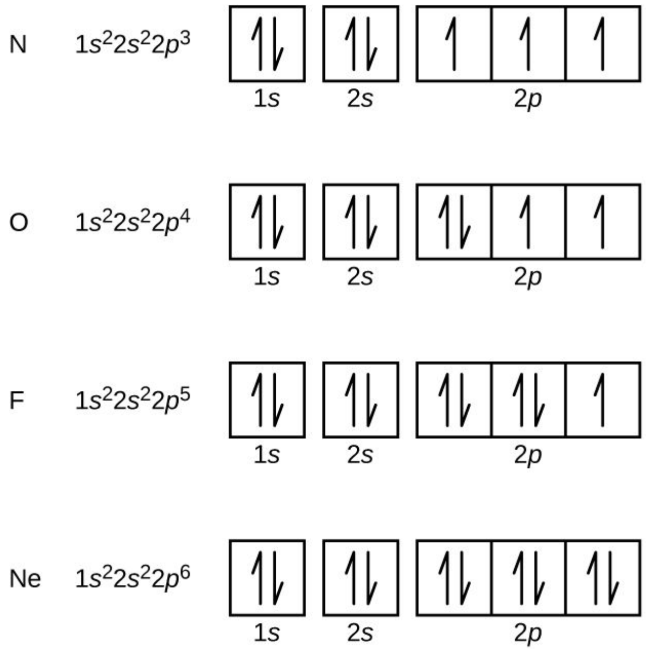
$[Kr]5s^1$

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

$[Xe]6s^2 4f^{14} 5d^{10} 6p^5$

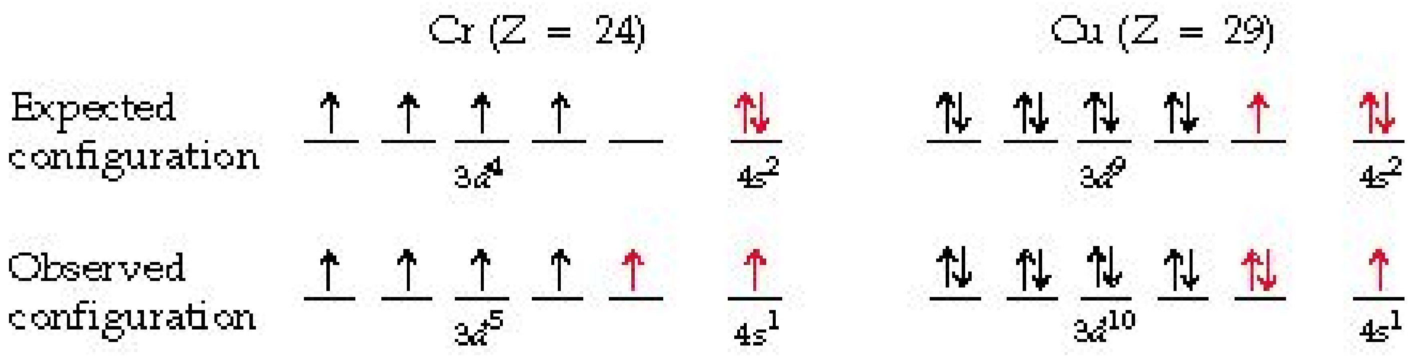
Electron Configurations

- Orbital diagrams: make use of arrows in boxes



Electron Configuration Exceptions

- A completely full or half full d sublevel is more stable than a partially filled d sublevel
- For Cu and Cr, an electron from the 4s orbital is excited and rises to a 3d orbital.



Main

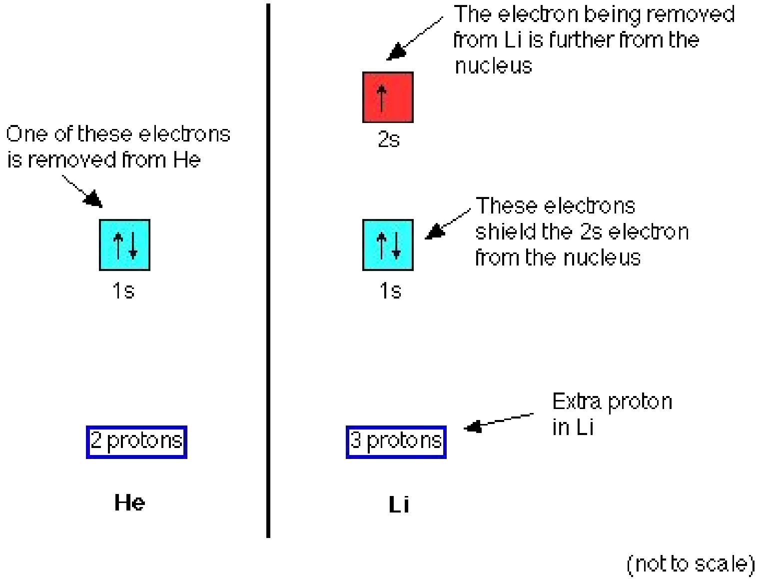
Lesson 4

Electrons in Atoms

Main

Emission Spectra and Ionization

- Ionization energy is the energy required to remove an electron from a neutral gaseous atom or molecule in its ground-state



Main

Emission Spectra and Ionization

- Trends in first ionization energy across periods account for the existence of main energy levels and sublevels in atoms.
- Successive ionization energy data for an element give information that shows relations to electron configurations.

Emission Spectra and Ionization

- First Ionization Energy:
  - $X(g) \rightarrow X^{+}(g) + e^{-}$
- Second Ionization Energy:
  - $X^{+}(g) \rightarrow X^{2+}(g) + e^{-}$
- n^{th} Ionization Energy:
  - $X^{(n+1)+}(g) \rightarrow X^{n+}(g) + e^{-}$

$$IE_1 < IE_2 < IE_3 < IE_4 \ldots$$

Calculating Ionization Energy

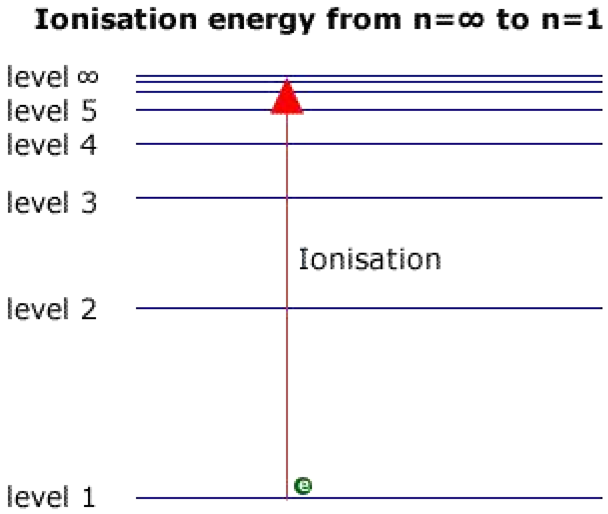
- Solve for energy

$$E = h\nu = \frac{hc}{\lambda}$$

- Multiply by Avogradro's constant to get the energy required to remove one mole (J mol^{-1})

Convergence

- At the limit of convergence the lines merge forming a continuum
- Beyond this continuum the electrons can have any energy; the electron is outside of the atom and ionization has occurred



Periodic Trends in Ionization Energies

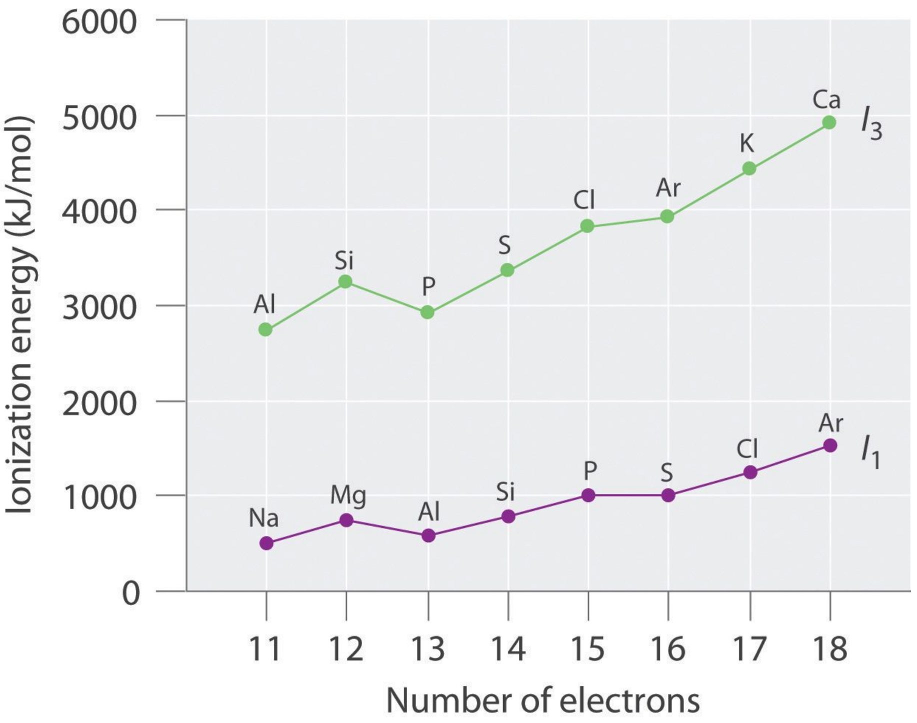


TABLE 7.2 **Successive Values of Ionization Energies, *I*, for the Elements Sodium Through Argon (kJ/mol)**

Element	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	496	4560					
Mg	738	1450	7730				
Al	578	1820	2750	11,600			
Si	786	1580	3230	4360	16,100		
P	1012	1900	2910	4960	6270	22,200	
S	1000	2250	3360	4560	7010	8500	27,100
Cl	1251	2300	3820	5160	6540	9460	11,000
Ar	1521	2670	3930	5770	7240	8780	12,000

(Inner-shell electrons)

Ionization of Unknown Element

- The first seven ionization energies of an unknown element are given. Which group might this element come from?

	1st	2nd	3rd	4th	5th	6th	7th
IE	1005	2260	3375	4565	6850	8490	27,000

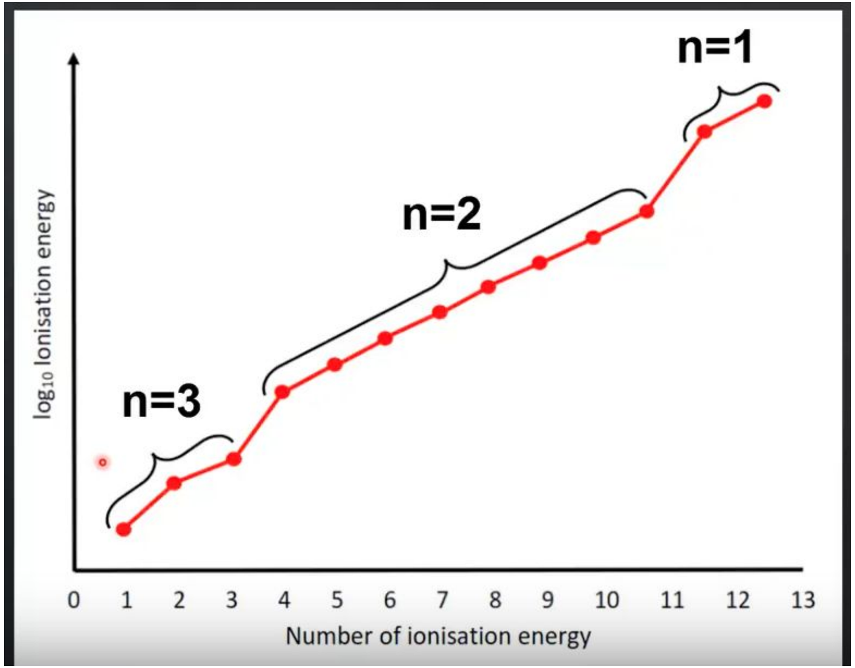
Ionization of Unknown Element

- There is a large jump from the 6th to the 7th ionization energies. The element is found in the 6th group.

	1st	2nd	3rd	4th	5th	6th	7th
IE	1005	2260	3375	4565	6850	8490	27,000

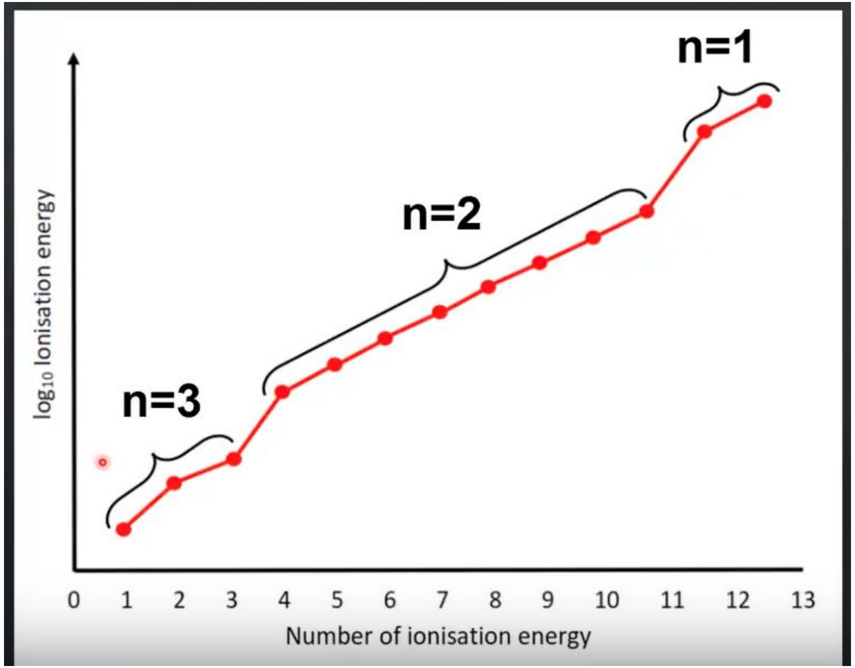
Successive Energy Levels

- Aluminum
  - $1s^2 2s^2 2p^6 3s^2 3p^1$
- The electrons are removed from the energy level farthest from the nucleus (n=3)
- Electrons in the outer energy level require less energy to remove because they are further away from the nucleus



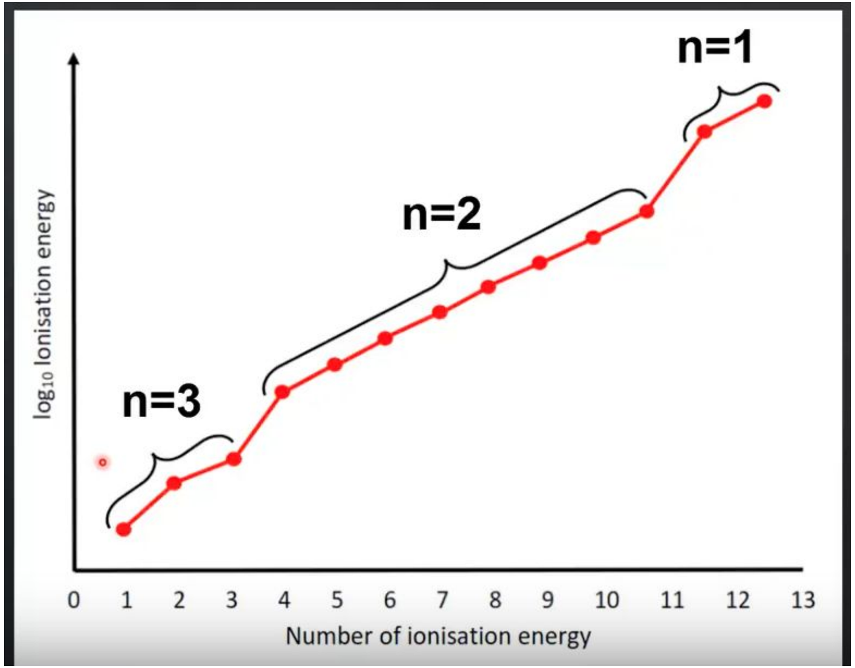
Successive Energy Levels

- Aluminum
  - $1s^2 2s^2 2p^6 3s^2 3p^1$
- The electrons are removed from the second energy level (n=2)
- The jump in ionization energy from the 3rd and 4th ionization energies is evidence of the existence of energy levels within the atom



Successive Energy Levels

- Aluminum
  - $1s^2 2s^2 2p^6 3s^2 3p^1$
- The electrons are removed from the energy level closest to the nucleus (n=1)
- Electrons in the inner energy level require more energy to remove because they are closer to the nucleus
- The jump in ionization energy from the 11th and 12th ionization energies is evidence of the existence of energy levels within the atom



Successive Energy Levels

- Aluminum
  - $1s^2 2s^2 2p^6 3s^2 3p^1$
- The larger ionization energy between the 9th and 10th value occurs because the 10th electron is removed from the 2s sublevel which experiences a stronger electrostatic attraction from the nucleus
- Provides evidence of sublevels in atoms