Chemistry 3A

Introductory General Chemistry

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Concepts

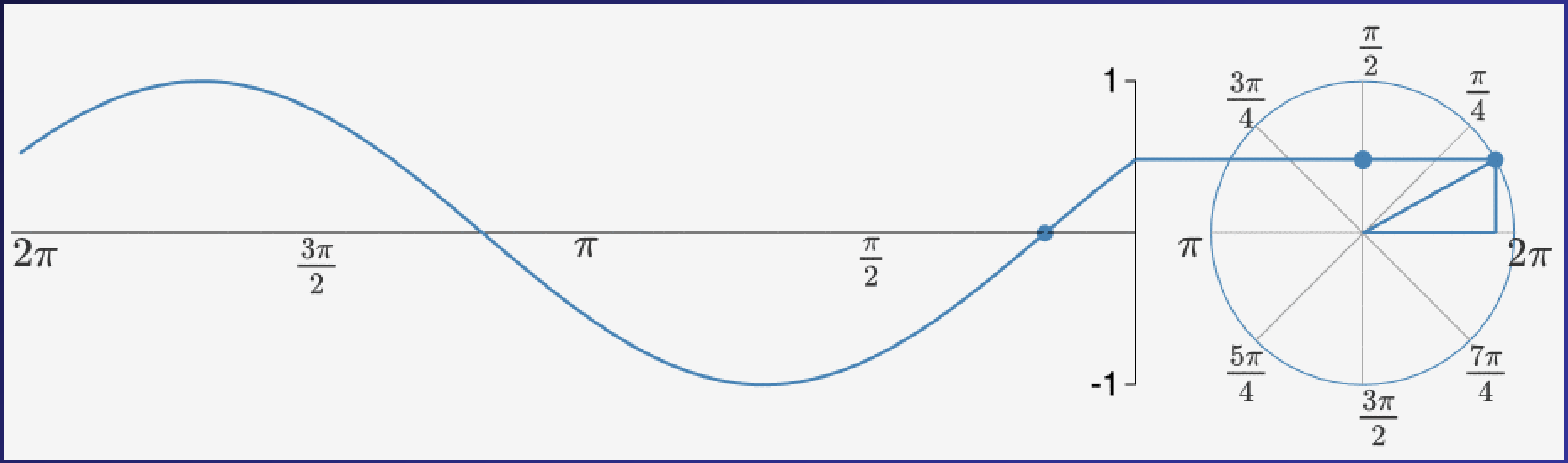
- Waves
- Observations on Atom Structure
- Electromagnetic Radiation & Spectrum
- Quantized Nature of Energy
- Energy levels of Electrons
- Quantum Mechanical Model of Atom
- Electron "Identity": Quantum Numbers
- Shells, Subshells
- Orbitals and their "Shapes"
- Populating (Filling) Electrons: Electron Configuration
- Related Trends in Periodic Table
- Atomic Radius, Ionization Energy, Electron Affinity

Waves

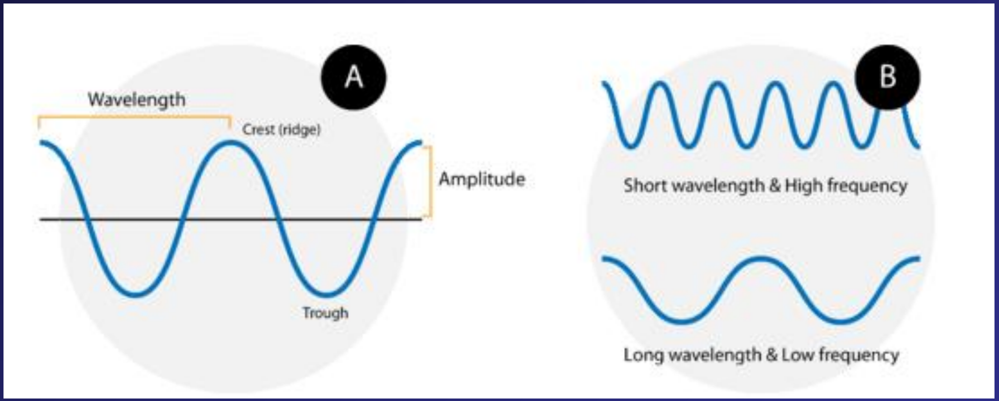
- Waves are a sinusoidal motion or movement

There are terms used to talk about waves

- Crest – the topmost point of a wave
- Trough – the bottommost point of a wave



Waves



Wavelength

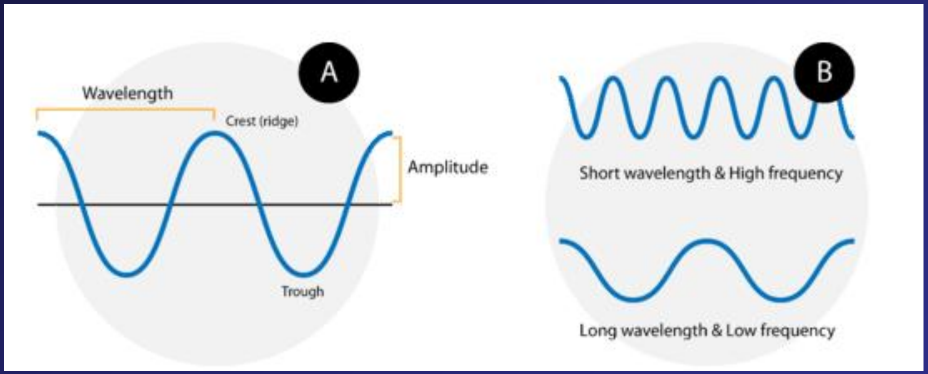
- Distance between to corresponding points on adjacent waves
- Crest-to-crest or trough-to-trough distance
- Represented by Greek letter *lambda* (λ)
- Units: some form of meter (m, nm, cm, km)

Frequency

- The number of waves that pass a point in a certain period of time
- Represented by Greek letter *nu* (ν)
- Units: per unit time [waves per second (s^{-1})]

  Also called Hertz (Hz)

Waves



Amplitude

- maximum distance or displacement of a wave from its resting (zero) position

  Also called equilibrium position
- represents height of wave's crest (or trough)
- indicator of the energy of a wave

  higher amplitude → higher energy

Wave speed

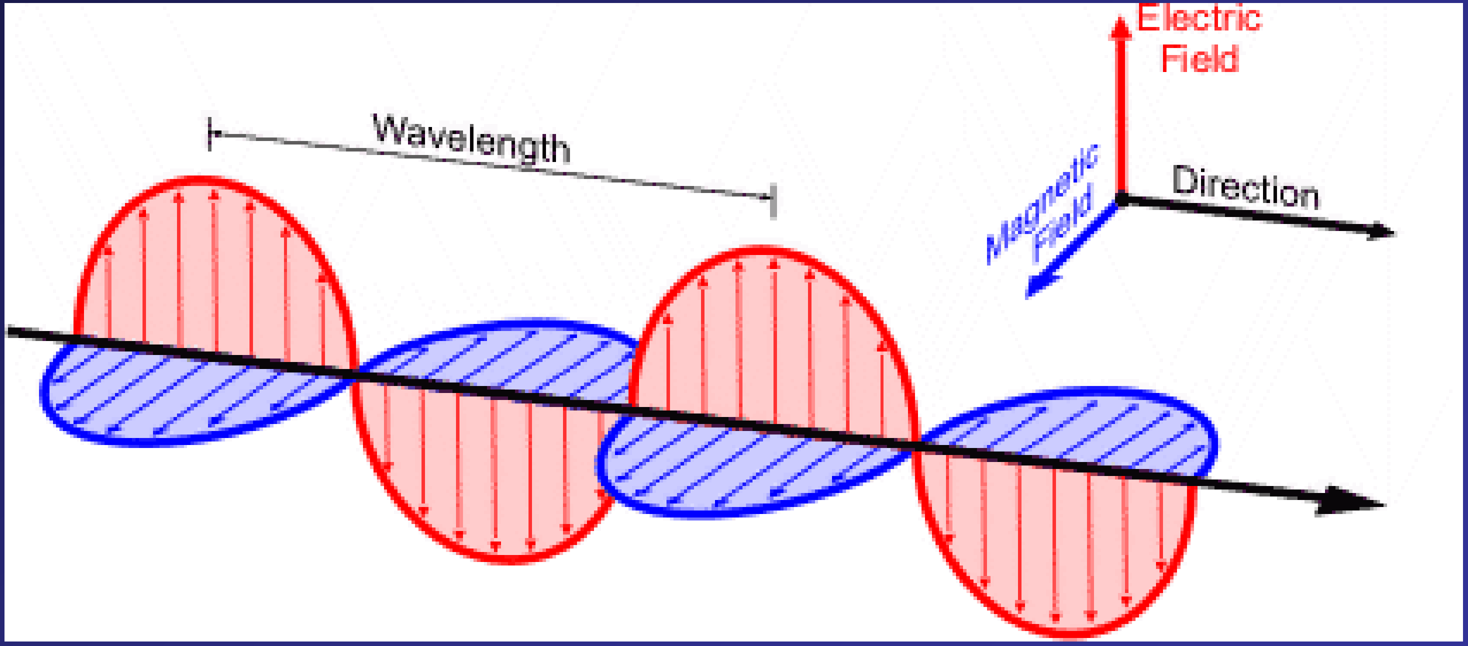
- distance a wave disturbance travels through a medium in a given amount of time
- Units: distance per unit time (m/s)
- indicated usually by ***v*** (velocity)

$$\text{wave speed} = \text{wavelength (m)} \times \text{frequency } (\text{s}^{-1})$$

$$v = \lambda \nu$$

Waves

- Electromagnetic radiation is a wave
- Actually a wave with two components perpendicular (at right angles, 90° to) each other
  - Electric field wave
  - Magnetic field wave



Waves

It is typical to talk about EM waves with respect to their wavelength

Frequency is required when you make energy calculations—*slide after next slide*!

In the visible light spectrum, wavelengths are from 400-700 nanometers (nm).

Color	Wavelength	Description
Red	~650 nm	Longest visible wavelength; warm and low-energy.
Green	~530 nm	Mid-spectrum; often associated with nature and balance.
Blue	~470 nm	Shorter wavelength; cooler and higher-energy.

Making A Calculation

What is the frequency of green light at 530 nm?

$$c = \lambda v$$

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

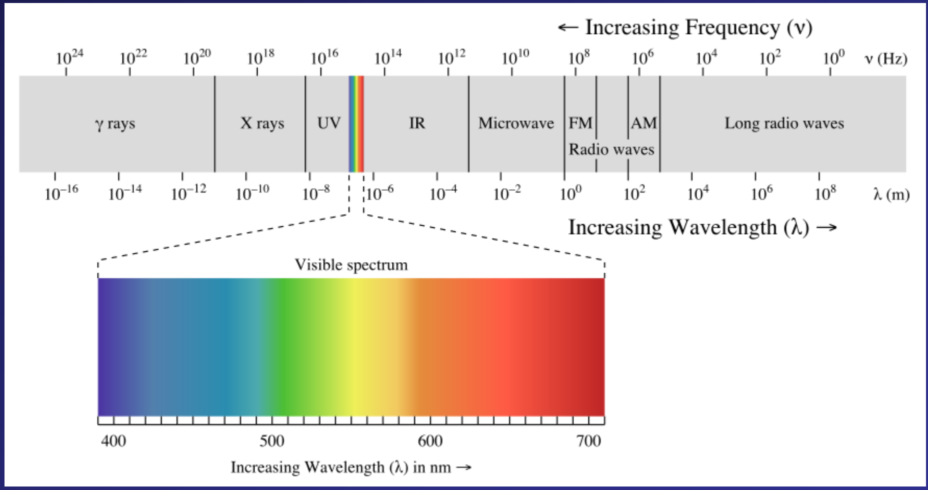
$$v = \frac{3.00 \times 10^{8}\ \text{m}}{\text{s}} \times \frac{1}{530\ \text{nm}} \times \frac{10^{9}\ \text{nm}}{1\ \text{m}} = 5.66 \times 10^{14}\ \text{s}^{-1}$$

or 5.66×10^{14} Hz

Algebra + conversion factors +
a natural constant (the speed of light)

Electromagnetic Spectrum

- Spans from radio waves to gamma rays
- Our eyes detect a narrow part of the EM spectrum called "visible light"



EM radiation has ENERGY that is calculated using the famous Planck's equation

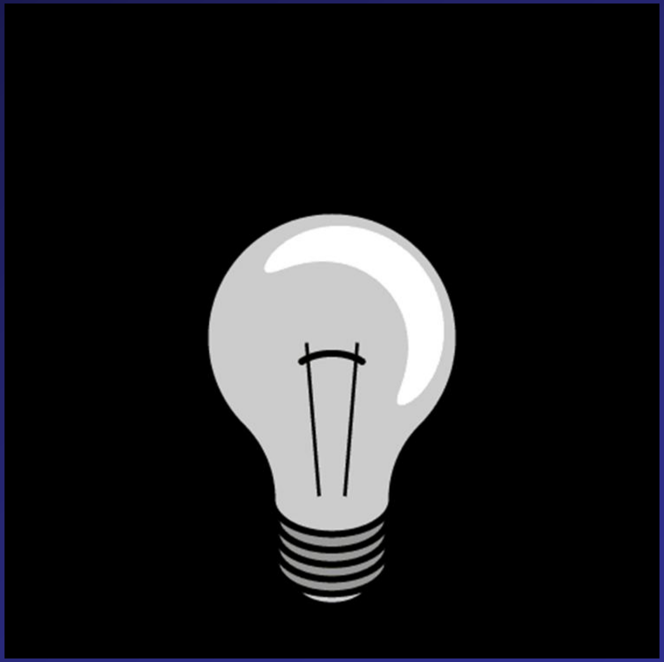
$$E = h\nu$$

EM radiation that is "ionizing" has frequencies in the UV and higher (X-rays, γ rays)

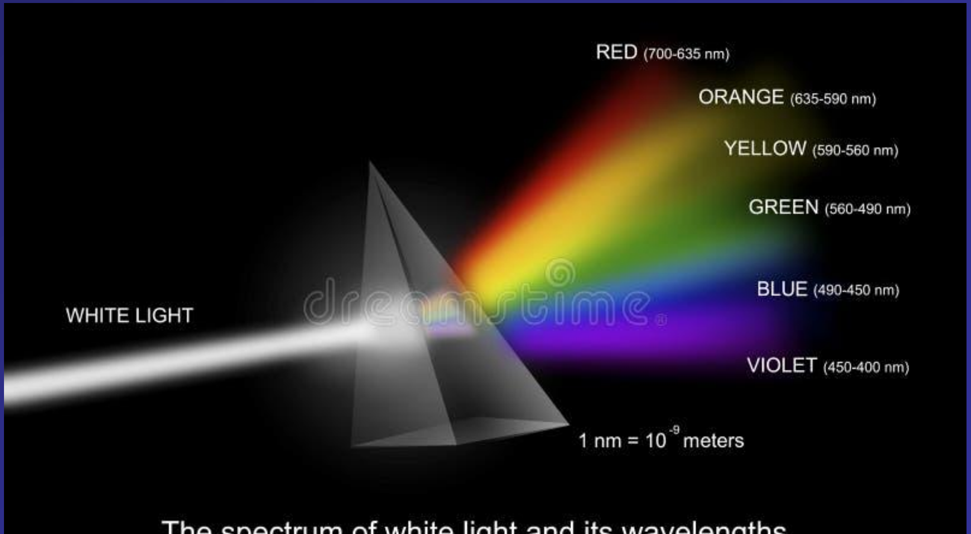
The Light Bulb

- An electric current passes through the tungsten filament

  Element symbol W
- The filament resists the flow, heating to ~3000 °C
- At this high temperature, it emits blackbody radiation
- The spectrum spans visible wavelengths, so the glow appears white light



⚡ This is not from tungsten’s atomic emission spectrum

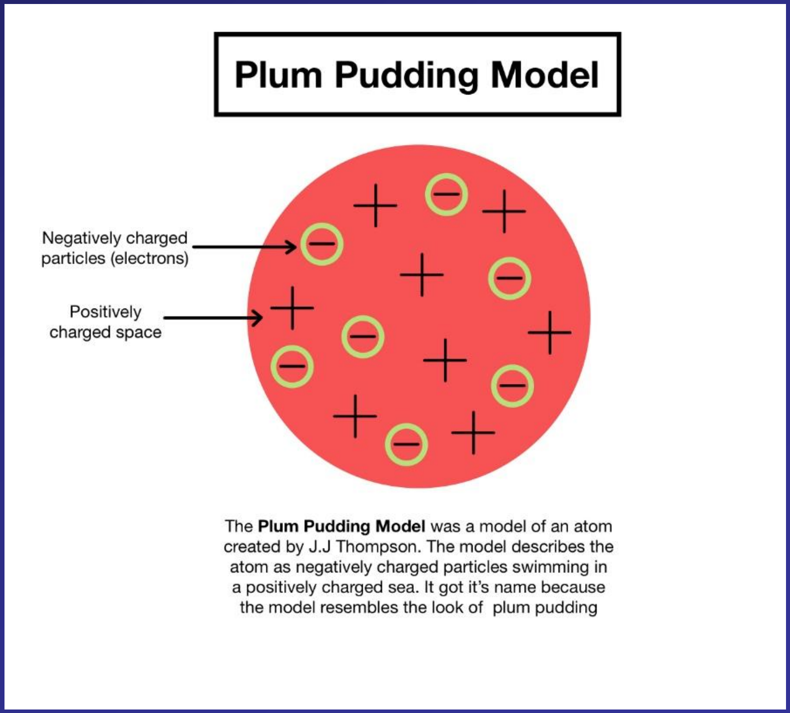


The spectrum of white light and its wavelengths

Historical Observations

- 1897 JJ Thomson discovers the electron is a negatively charged particle
- Proposes "plum pudding" model of atom

- Electrons and protons in a mix (cloud)
- No nucleus



Historical Observations

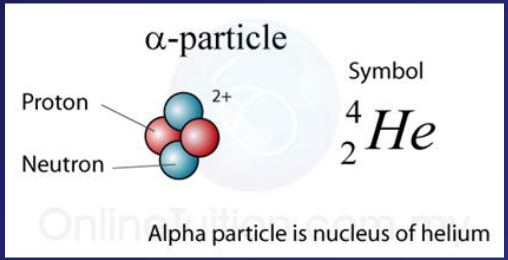
1909 Rutherford aimed alpha particles at thin gold foil and he sees that they pass through the foil and some are deflected

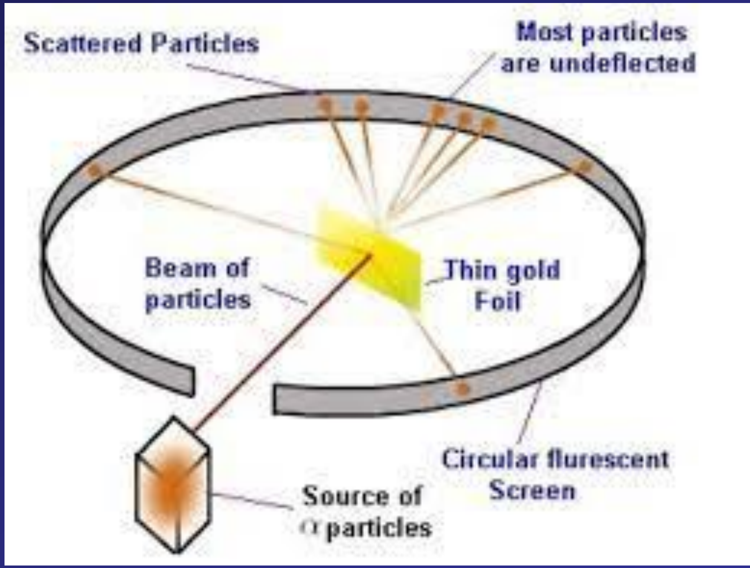
Alpha particles are positively charged helium atoms (^{4}He)

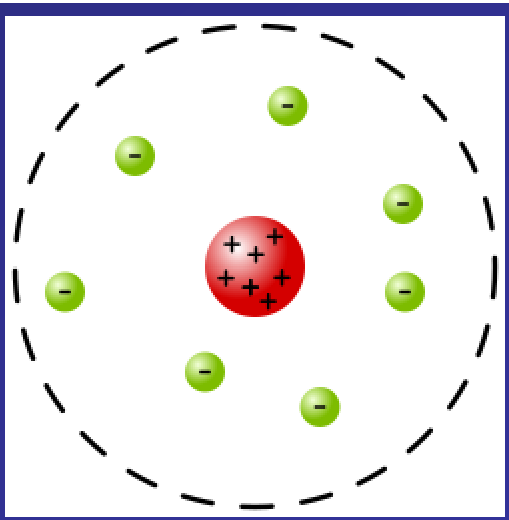
Important findings

- Gold foil atoms must have space in them or the alpha particles would not pass through
- The deflections would have to be positive charges in the gold foil, since positive charges repel

Rutherford proposes a positively charged “nucleus” with electrons outside of it (did not describe orbits)



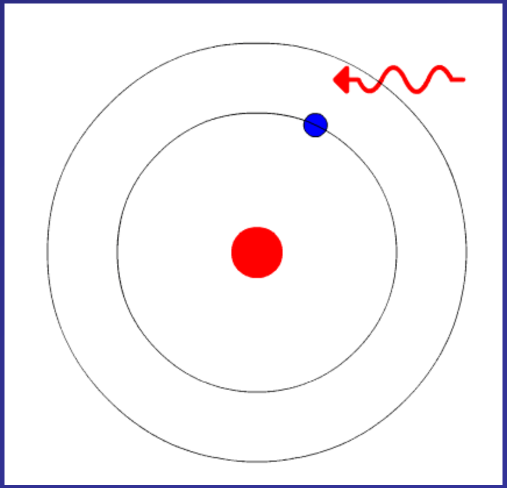




Atoms & Orbiting Electrons

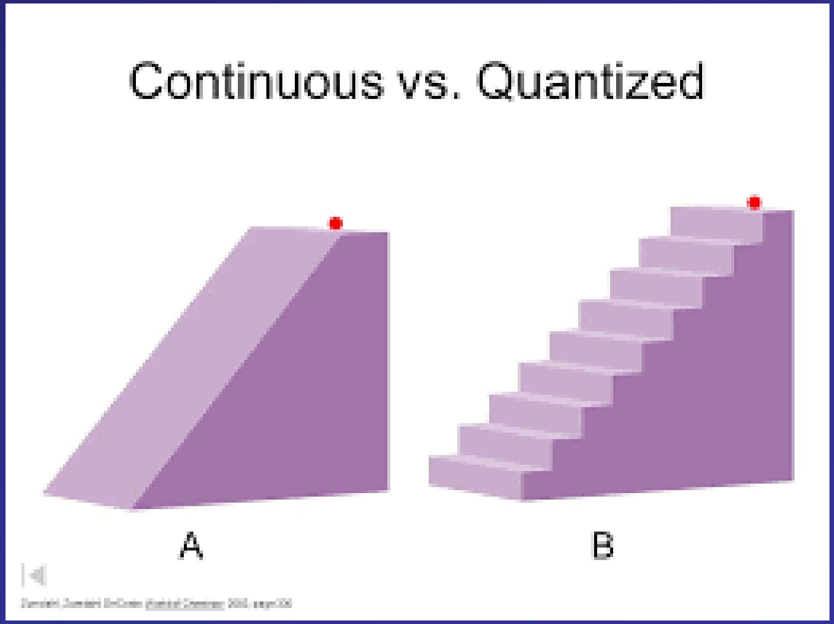
The Bohr Model

- Electrons orbit the nucleus in fixed energy levels
- Electrons can transition between energy levels by absorbing or emitting a photon as a quantum of energy
- Transition between a ground state and excited state
- Explained the hydrogen emission spectrum with mathematical precision



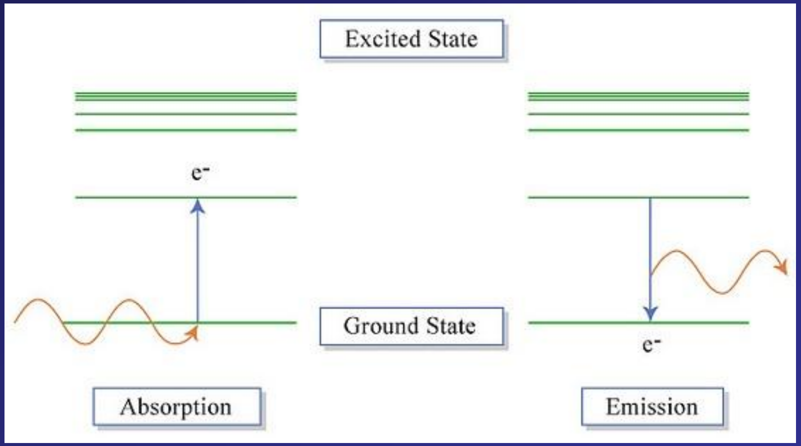
Quantized vs Continuous

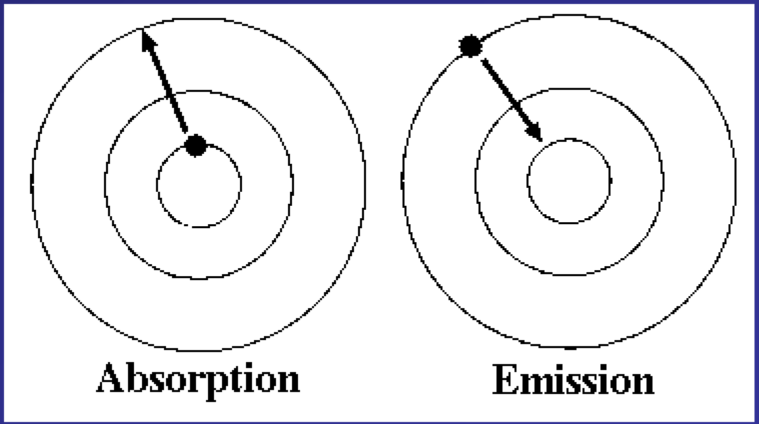
- Energy level transitions in atoms are quantized
- Electrons cannot absorb just any amount of energy
- They can only move between specific energy levels with exact energy differences
- If incoming photon does not have required amount of energy, no transition occurs



Electrons & Energy Levels

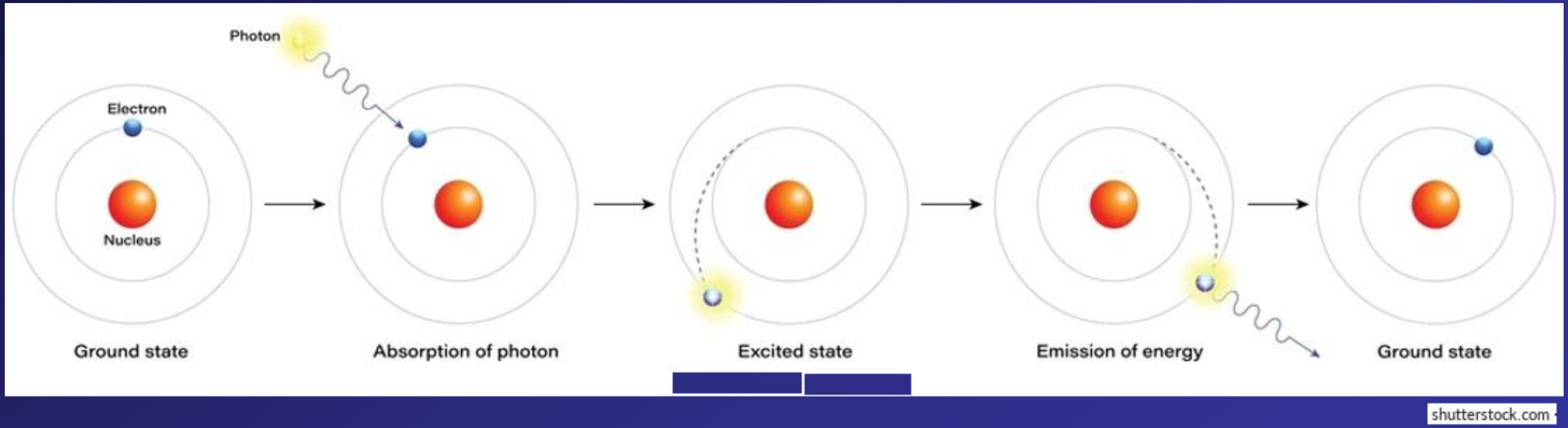
- An electron in an atom moves in an orbit about the nucleus of the atom
- Its usual orbit is in a ground state, its lowest energy state
- When given energy through the "absorption" of a photon (EM radiation), it jumps to another a higher energy level, an orbit further away from the nucleus. It is in an excited state.
- When it loses its energy back to its ground state, it emits a photon.





Electrons and EM Radiation

- This cycle of absorbing photon in the ground state and being excited (the excited state) to an energy level and then relaxing or losing that energy back to the ground state with emission of a photon shown below



Emission Spectrum

These electron energy level transitions explain the emission spectra observations

- Hydrogen atom has only a few energy transitions
- Iron atom has numerous of these transitions

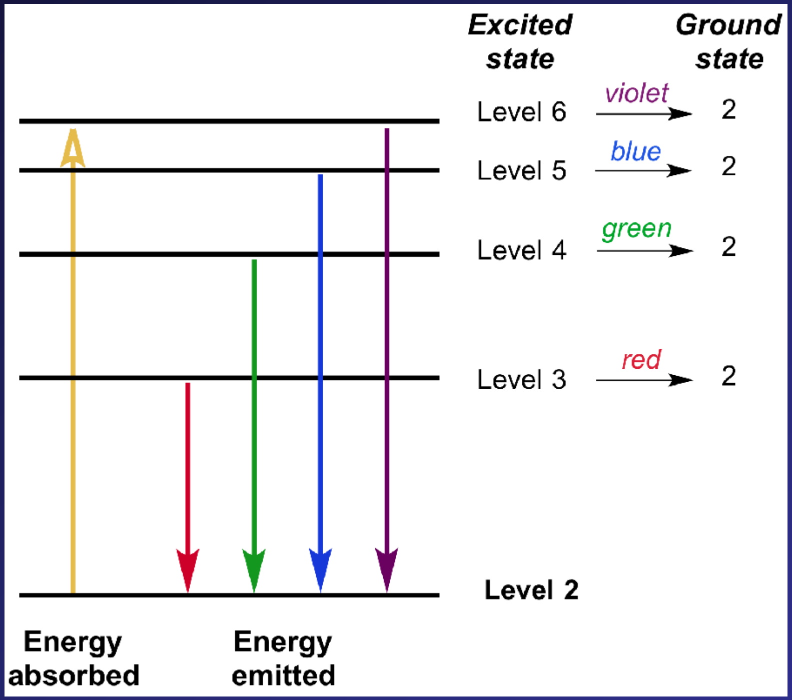


Figure 3.2.1.2: Atomic Emission Spectrum of Hydrogen.

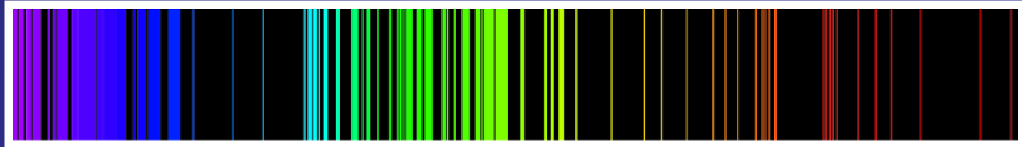
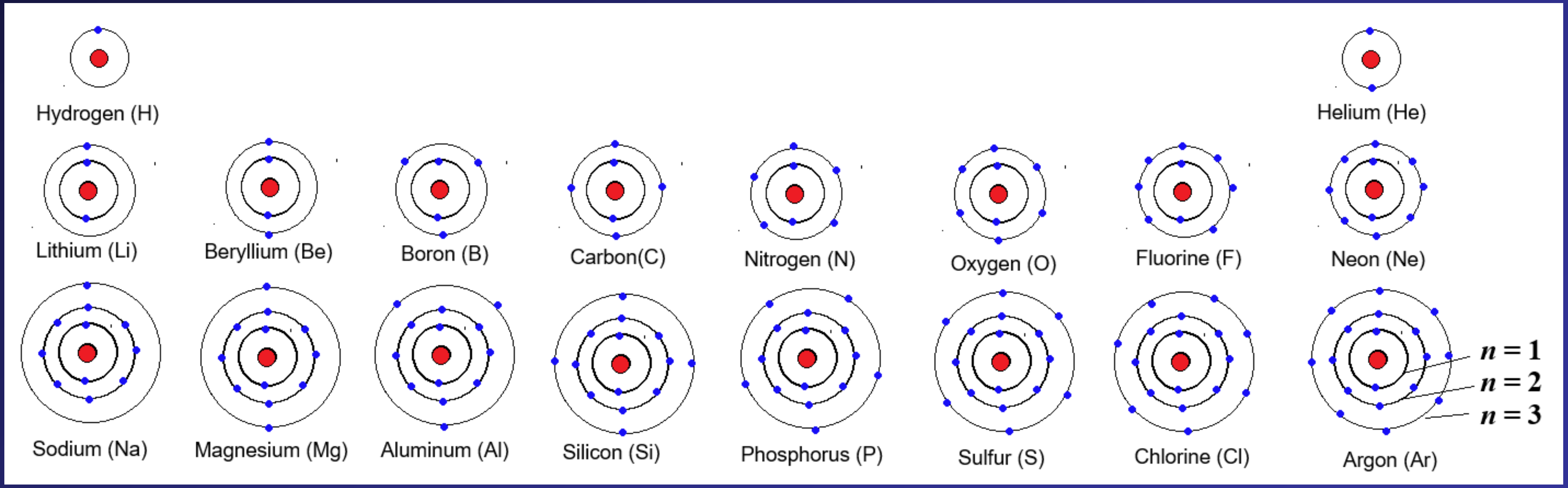


Figure 3.2.1.3: Atomic Emission Spectrum of Iron.

Quantum Mechanics Model

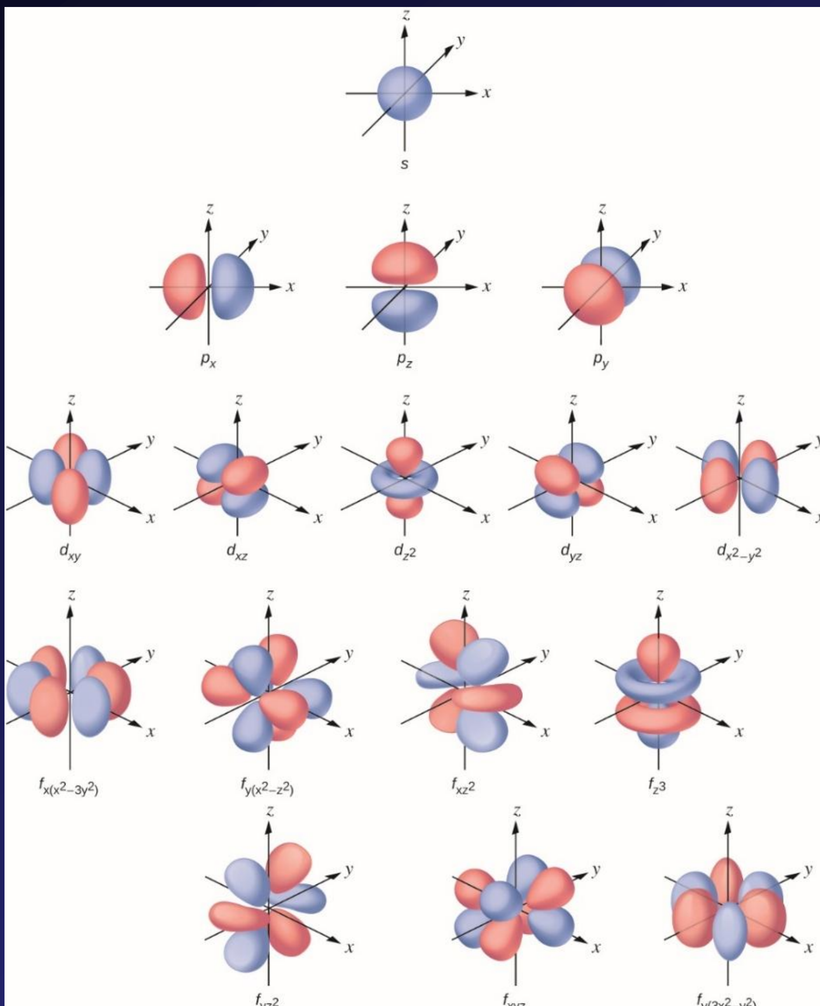
- Following Bohr's explanations, a model for how electrons exist
- Electrons have an identity: quantum numbers
- There are 4 quantum numbers for each electron



Quantum Numbers: Meaning

- Principal Quantum Number (***n***)
  - describes main energy level or shell the electron is in
  - the bigger the number (1,2,3,...), the farther the electron is from the nucleus and the higher its energy
- Angular Momentum Quantum Number (***l***)
  - describes shape of the orbital, or the region where the electron is likely to be found
  - the shapes are given letter names (come from spectroscopy): *s* (sphere), *p* (dumbbell), *d* (cloverleaf), *f* (double cloverleaf)
- Magnetic Quantum Number (m_l)
  - Describes the orientation of the orbital in 3D space
  - For a dumbbell-shaped p-orbital, this number tells you if it's on the x, y, or z-axis
- Spin Quantum Number (m_s)
  - Describes an electron's intrinsic "spin"
  - There are only two possible values: spin up (+1/2) or spin down (−1/2)
  - Every orbital can hold a maximum of two electrons
  - They must have opposite spins

Orbitals and Electron Configurations



Orbital shapes are actually mathematical calculations describing the space where an electron can be found

- Probabilities functions

Depending on the value of ***n*** (the shell), there is possible

- only one *s* orbital
- three *p* orbitals
- five *d* orbitals
- seven *f* orbitals

Each orbital can have only two electrons

Orbitals and Electron Configurations

Table 3.3.1: Atomic shell and subshell structure with the number of electrons in each

Shell	Number of Subshells	Names of Subshells	Number of Orbitals (*per Subshell*)	Number of Electrons (*per Subshell*)	Total Electrons (*per Shell*)
1	1	*1s*	1	2	2
2	2	*2s* and *2p*	1, 3	2, 6	8
3	3	*3s, 3p,* and *3d*	1, 3, 5	2, 6, 10	18
4	4	*4s, 4p, 4d,* and *4f*	1, 3, 5, 7	2, 6, 10, 14	32

Why these patterns in this detail?

- Because it explains the nature of the atoms and Periodic Table
- It explains the ***periods*** (rows) and the ***groups*** (columns)
- This will be an exercise in memorization of these patterns of matter, nature, and the atom

Atomic Structure Glossary

Term	Definition	Symbol/Example
Shell	A major energy level in an atom, defined by principal quantum number ***n***. All electrons with same n are in same shell	***n*** = 1, 2, 3, …
Subshell	Subdivision of shell defined by the azimuthal quantum number ***l***. Determine the shape of the orbital	***l*** = 0 (***s***), ***l*** = 1 (***p***), ***l*** = 2 (***d***), ***l*** = 3 (***f***)
Energy Level	Used synonymously with ***shell*** (but can refer to quantized energy associated with electron's position in atom	Can also refer to ground state vs excited state
Energy Sublevel	Informal term for ***subshell*** and it emphasizes the energy hierarchy within a shell	*3s* < *3p* < *3d* (within shell ***n*** = 3)
Orbital	A region of space where there is high probability of finding an electron. Defined by (n, l, m_l)	Examples: $2p_x$, $3d_{xy}$

Quantum Number Relationships

More info for emphasis

Shell → defined by n

Subshell → defined by n and l

Orbital → defined by n, l , m_l

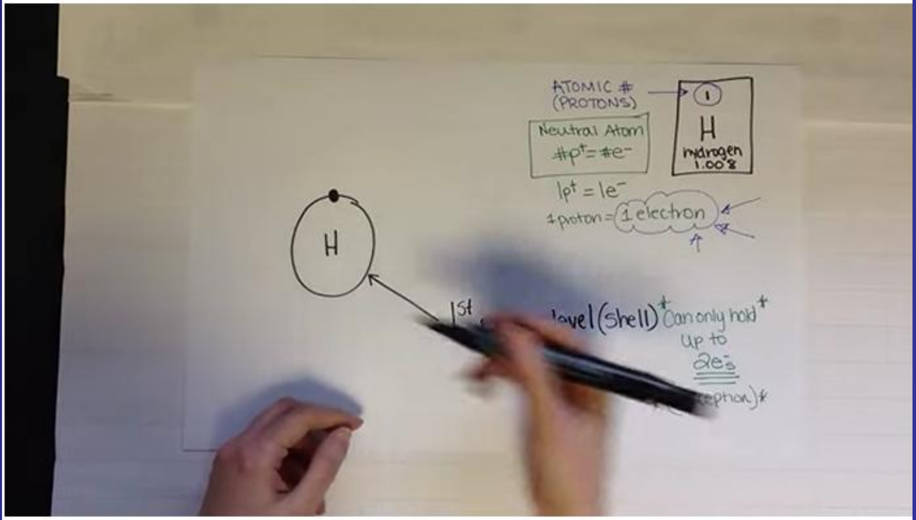
Electron spin → defined by m_s, either $+½$ or $-½$

This use of many terms
is indicated to you because
a 9-minute video in your
book also uses certain terms

Visual Analogy

Think of it like a building:

- **Shell** = floor number
- **Subshell** = room type (s, p, d, f)
- **Orbital** = specific room
- **Electron** = person in the room, with spin direction like facing left or right

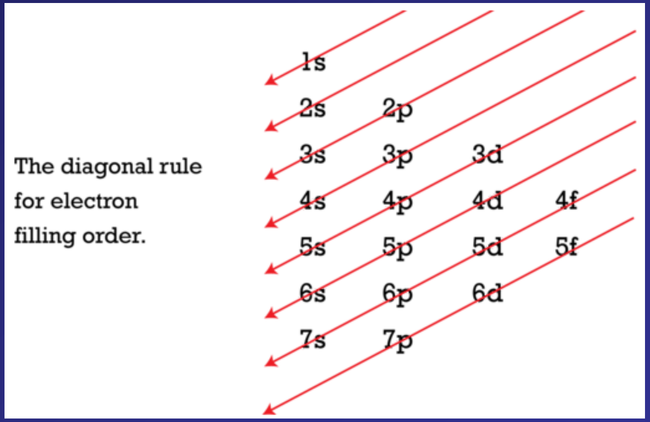


Video 3.3.1: Energy levels, sublevels and orbitals.

Orbital Filling

Aufbau Principle

In "filling" the atom's orbitals so that electron's are added in order of lowest to higher energy, use the $n + l$ Aufbau Principle. <u>The lower value gets filled first</u> ("Aufbau" is "build up" in German)



WAIT!!

Shouldn't $n = 4$ have higher energy level than $n = 3$, so why fill ***4s*** before ***3d*** !!??

Well…it's really $n + l$

$4s = 4 + 0 = 4$

$3d = 3 + 2 = 5$

So ***4s*** gets filled first

shape	l
s	0
p	1
d	2
f	3

Quantum Number Uniqueness

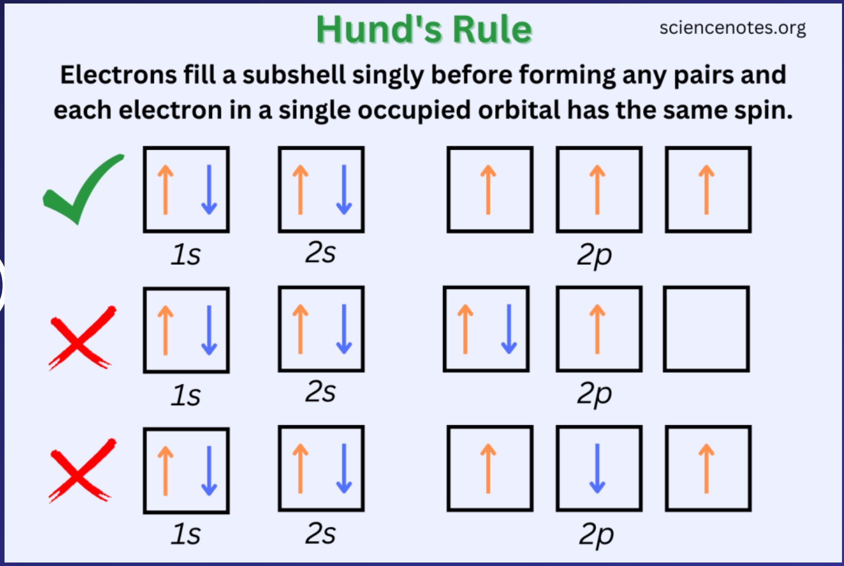
Pauli Exclusion Principle

Remember those four quantum numbers that indicate the "identity" of an electron in the atom?

The Pauli Exclusion Principle is just a rule that states that no two electrons in an atom can have the same four quantum numbers, the same "identity"

Unpaired vs Paired Electrons

Hund's Rule



- Electrons can be "paired" into orbitals (2 e^- per orbital)

  They must have opposite spins
- But pairing requires an energy input
- For orbitals of the same energy level (degenerate orbitals), fill the orbitals FIRST with one electron, and as filling proceeds, then pair them
- This applies to *p* (3 degenerate orbitals), *d* (5), and *f* (7). The *s* orbital has only one energy level

Electron Configurations

- The electrons that will complete a particular atom are presented in a particular format called an electron configuration
- The format is

<***n***-number><***l***-letter>$^{\text{<\# of electrons superscript>}}$

The ***n***-number will be shell number: 1, 2, 3, 4, 5, 6, 7

The ***l***-letter will be subshell designation: ***s, p, d, f***

The # of electrons in superscript are the range of electrons possible for the subshell: *s* → 1 × 2 = 2 , *p* → 3 × 2 = 6, *d* → 5 × 2 = 10, *f* → 7 × 2 = 14

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4	4	*4s*, *4p*, *4d*, and *4f*	1, 3, 5, 7	2, 6, 10, 14	32

Electron Configurations

- Actual electron configuration in 2nd column
- The 3rd column shows the filling of orbitals according to Hund's Rule

Hydrogen	$1s^1$	
Helium	$1s^2$	
Lithium	$1s^22s^1$	
Beryllium	$1s^22s^2$	
Boron	$1s^22s^22p^1$	$1s^22s^22p_x^1$
Carbon	$1s^22s^22p^2$	$1s^22s^22p_x^1p_y^1$
Nitrogen	$1s^22s^22p^3$	$1s^22s^22p_x^1p_y^1p_z^1$
Oxygen	$1s^22s^22p^4$	$1s^22s^22p_x^2p_y^1p_z^1$
Fluorine	$1s^22s^22p^5$	$1s^22s^22p_x^2p_y^2p_z^1$
Neon	$1s^22s^22p^6$	$1s^22s^22p_x^2p_y^2p_z^2$

Core and Valence Electrons

- The outermost shell (shells designated by the ***n*** value) of the atom contains electrons called the valence electrons
- All other (inner) shells form the core electrons

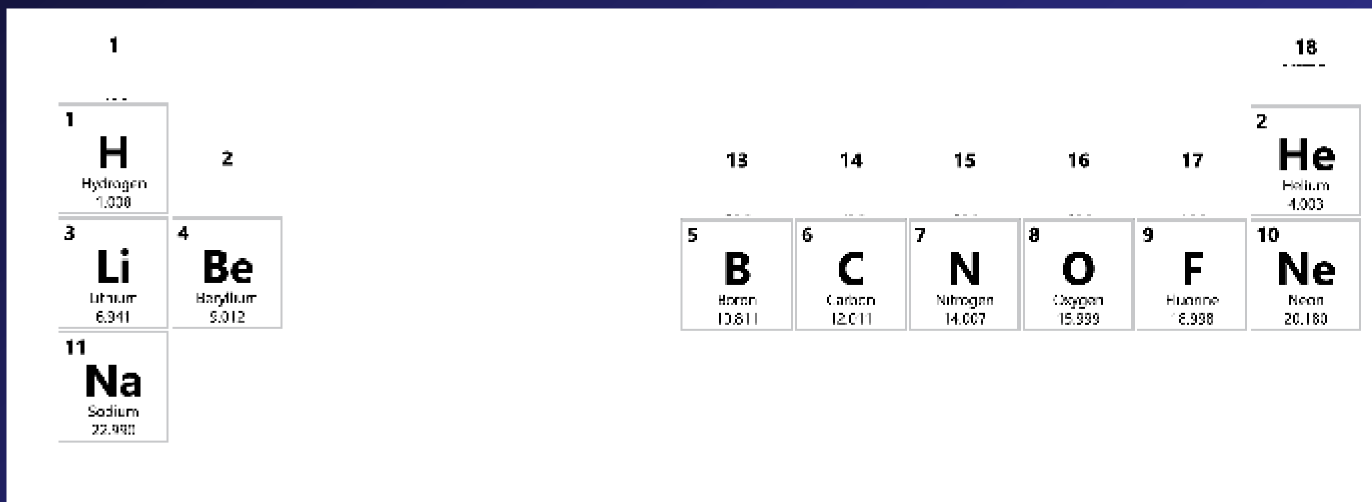


Figure 3.4.1: A core-abbreviated electron configuration (right) replaces the core electrons with the noble gas symbol whose configuration matches the core electron configuration of the other element.

Electron Configurations

Hydrogen (H)	$1s^1$	Iron (Fe)	$[Ar]3d^64s^2$
Helium (He]	$1s^2$	Copper (Cu)	$[Ar]\ 3d^{10}4s^1$
Lithium (Li)	$[He]2s^1$	Zinc (Zn)	$[Ar]4s^23d^{10}$
Boron (B)	$[He]2s^22p^1$	Silver (Ag)	$[Kr]5s^14d^{10}$
Carbon (C)	$[He]2s^22p^3$	Platinum (Pt)	$[Xe]4f^{14}5d^96s^1$
Sodium (Na)	$[Ne]3s^1$	Gold (Au)	$[Xe]\ 4f^{14}5d^{10}6s^1$
Magnesium (Mg)	$[Ne]3s^2$	Mercury (Hg)	$[Xe]\ 4f^{14}5d^96s^1$

- Copper: (move 4*s* electron to 3*d*!) making $3d^{10}4s^1$ is more energetically stable than expect $3d^94s^2$
- Zinc: not a transition metal (!) according to IUPAC
- Silver: like copper in filling the *d*-subshell
- Platinum: big exception in stabilizing 5*d* subshell
- Gold: Move from 6*s* to 5*d* completes the 5*d* subshell!

Exceptions to Rules Always

Notice an electron is taken from *4s* and put into *3d* for some of the elements!

It's always about a more energetically stable configuration

Element	Atomic Number	Electron Configuration	Notes
Scandium (Sc)	21	[Ar] $4s^2\ 3d^1$	First transition metal
Titanium (Ti)	22	[Ar] $4s^2\ 3d^2$	Follows Aufbau strictly
Vanadium (V)	23	[Ar] $4s^2\ 3d^3$	
Chromium (Cr)	24	[Ar] $4s^1\ 3d^5$	⚠️ Exception: half-filled d^5 is more stable
Manganese (Mn)	25	[Ar] $4s^2\ 3d^5$	
Iron (Fe)	26	[Ar] $4s^2\ 3d^6$	
Cobalt (Co)	27	[Ar] $4s^2\ 3d^7$	
Nickel (Ni)	28	[Ar] $4s^2\ 3d^8$	
Copper (Cu)	29	[Ar] $4s^1\ 3d^{10}$	⚠️ Exception: full d^{10} is more stable
Zinc (Zn)	30	[Ar] $4s^2\ 3d^{10}$	Not technically a transition metal by IUPAC

Second Period Elements

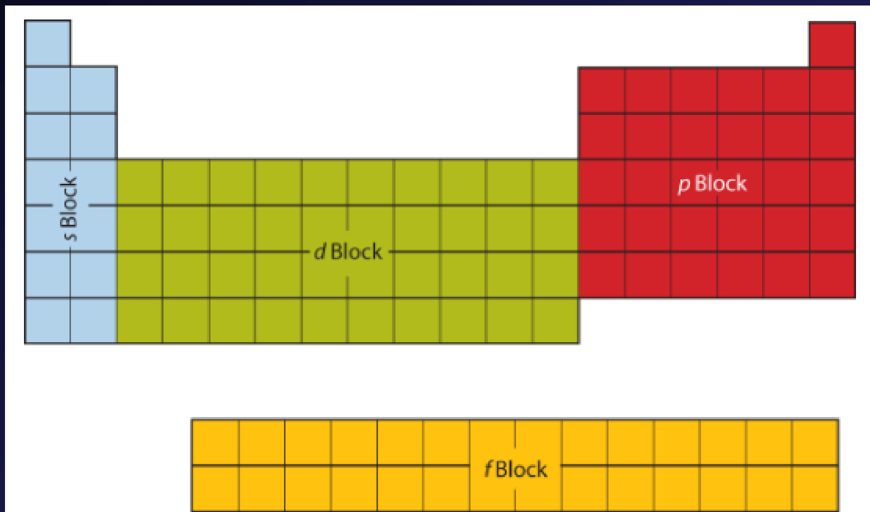
- 1st period has only two elements: hydrogen (H) and helium (He)
- 2nd period has 8 elements

Table 3.3.3: Electron Configurations of Second-Period Elements

Element Name	Symbol	Atomic Number	Electron Configuration
Lithium	Li	3	$1s^2\ 2s^1$
Beryllium	Be	4	$1s^2\ 2s^2$
Boron	B	5	$1s^2\ 2s^2\ 2p^1$
Carbon	C	6	$1s^2\ 2s^2\ 2p^2$
Nitrogen	N	7	$1s^2\ 2s^2\ 2p^3$
Oxygen	O	8	$1s^2\ 2s^2\ 2p^4$
Fluorine	F	9	$1s^2\ 2s^2\ 2p^5$
Neon	Ne	10	$1s^2\ 2s^2\ 2p^6$

- Along with hydrogen (H), 2nd period elements are the most important to life: carbon (C), nitrogen (N), oxygen (O)

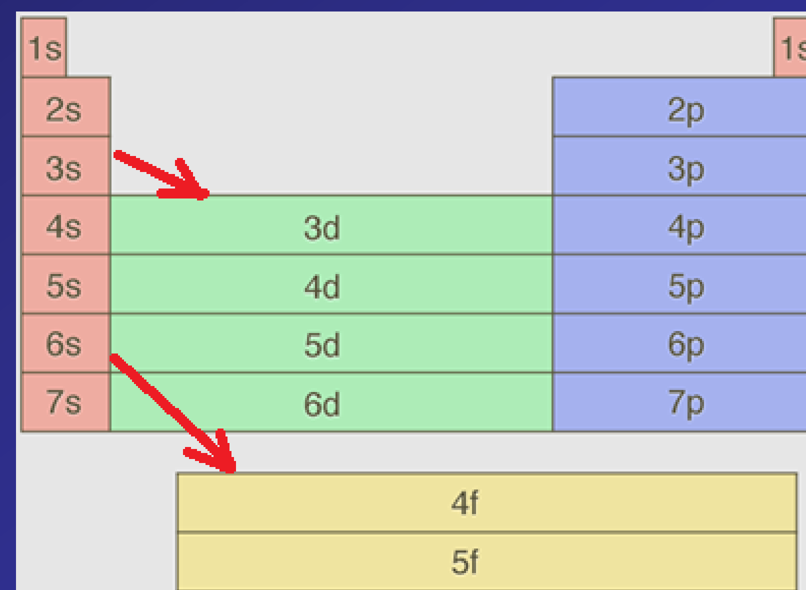
Electron Configurations and Periodic Table



- Subshells important
- *s* → 1 = 1 x 2e$^-$ = 2e$^-$
- *p* → 3 = 3 x 2e$^-$ = 6e$^-$
- *d* → 5 = 5 x 2e$^-$ = 10e$^-$
- *f* → 7 = 7 x 2e$^-$ = 14e$^-$

Note how ***3d*** is in the 4th period and ***4f*** actually starts in the 6th period!

Why??



The $n + l$ Rule (Aufbau Principle Reiterated)

Why does *3d* occur in the 4th period and *4f* occur in the 6th period?

1. Orbitals with lowest $n + l$ get filled first
2. If two orbitals have same $n + l$ the one with smaller n fills first

n
1
2
3
4
5
6
7

l	
s	0
p	1
d	2
f	3

4s (n =4, l =0) $\rightarrow n + l$ = 4

3d (n =3, l =2) $\rightarrow n + l$ = 5

4f (n =4, l =3) $\rightarrow n + l$ = 7

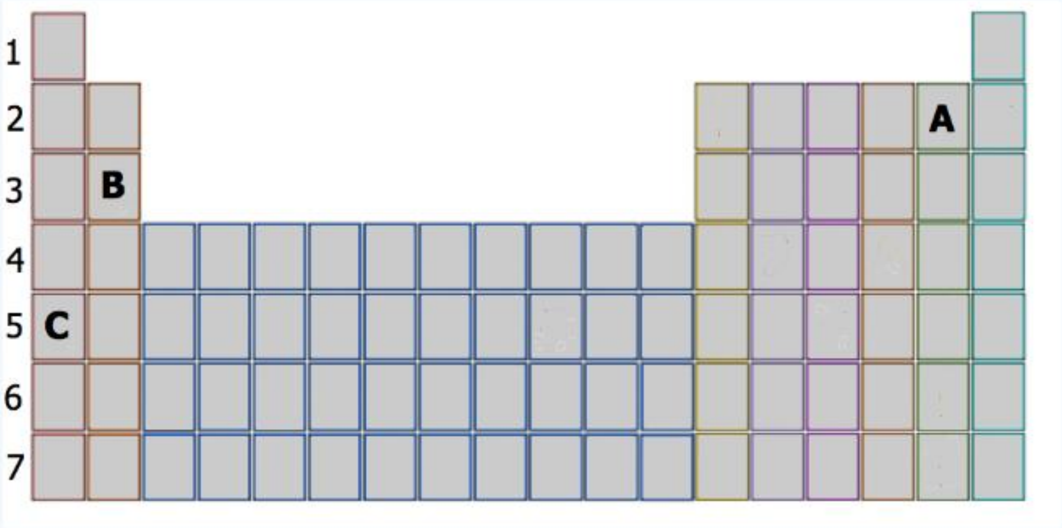
6s (n =6, l =0) $\rightarrow n + l$ = 6

Explains why *4s* fills before *3d*,

And *6s* before *4f*

Figuring Out Valence Electron Numbers

Based on their respective locations in the periodic table (use Figure 3.4.3), determine the number of valence electrons and the valence shell configuration of elements A, B and C.



Solution

Element A is located in Period 2, the *5th position* in *2p*-block. Before the electrons are placed in *2p* subshell, the *2s* subshell must be filled first. This means that A has ***two valence electrons*** in 2s (**$2s^2$**) and ***five valence electrons*** in 2p (**$2p^5$**). Answer: **$2s^22p^5$.** It has ***2 + 5 = 7*** **valence electrons.**

Element B is located in Period 3, the *2nd position* in *3s*-block. This means that B has ***two valence electrons*** in 3s (**$3s^2$**). Answer: **$3s^2$.**

Element C is located in Period 5, the *1st position* in *5s*-block). This means that there is only **one valence electron** in 5s (**$5s^1$**). Answer: **$5s^1$**.

Atomic Radius ("size")

- Going DOWN the table (1st, 2nd, … period), the radius INCREASES

***Adding shells** makes an atom bigger generally*

- Going RIGHT in table (1st,2nd … groups), the radius DECREASES

***Adding protons without adding a shell** pulls all electrons in closer to nucleus*

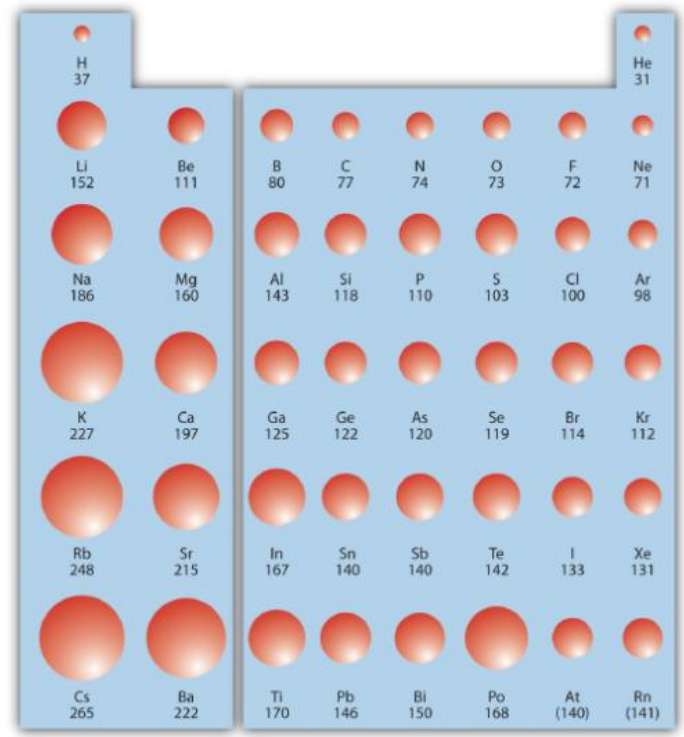


Figure 3.6.1: Atomic Radii Trends on the Periodic Table. Although there are some reversals in the trend (e.g., see Po in the bottom row), atoms generally get smaller as you go across the periodic table and larger as you go down any one column. Numbers are the radii in pm.

Ionization Energy

- Going DOWN the table (1^{st}, 2^{nd}, … period), the ionization energy DECREASES

Easier to remove one valence electron as valence shell gets further away from nucleus

- Going RIGHT in table (1^{st},2^{nd} … groups), the ionization energy INCREASES

Because radius decreases, valence electrons are brought in closer, so takes more energy to ionize

$$A(g) \rightarrow A^{+}(g) + e^{-} \qquad \Delta H \equiv IE$$

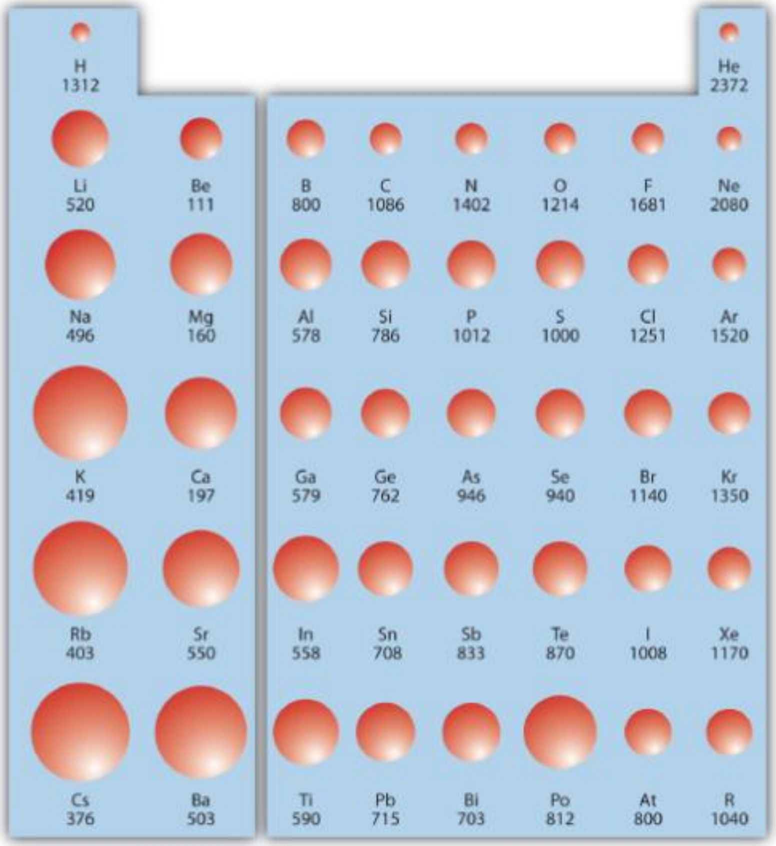


Figure 3.6.2: Ionization Energy on the Periodic Table. Values are in kJ/mol.

2^{nd}, 3^{rd},… Ionization Energies

- First Ionization Energy (IE_1) = 738 kJ/mol:

$$Mg(g) \rightarrow Mg^{+}(g) + e^{-}$$

- Second Ionization Energy (IE_2) = 1,450 kJ/mol:

$$Mg^{+}(g) \rightarrow Mg^{2+}(g) + e^{-}$$

- Third Ionization Energy (IE_3) = 7,734 kJ/mol:

$$Mg^{2+}(g) \rightarrow Mg^{3+}(g) + e^{-}$$

Removing additional electrons requires more energy because each ion becomes increasingly positive, strengthening its hold on remaining electrons. Electrostatic attraction grows, making further ionization energetically costly

Electron Affinity (EA)

$$A(g) + e^- \rightarrow A^-(g) \qquad \Delta H \equiv EA$$

- Going DOWN the table (1^{st}, 2^{nd}, … period), there appears to be no clear trend

As atom gets larger, they have more diffuse electron clouds: any added electron experiences weaker attraction to nucleus, so energy release less significant

- Going RIGHT in table (1^{st},2^{nd} … groups), the electron affinity INCREASES

Atoms strongly favor gaining electrons to complete the valence shell, and the added electron releases energy in stabilizing the atom

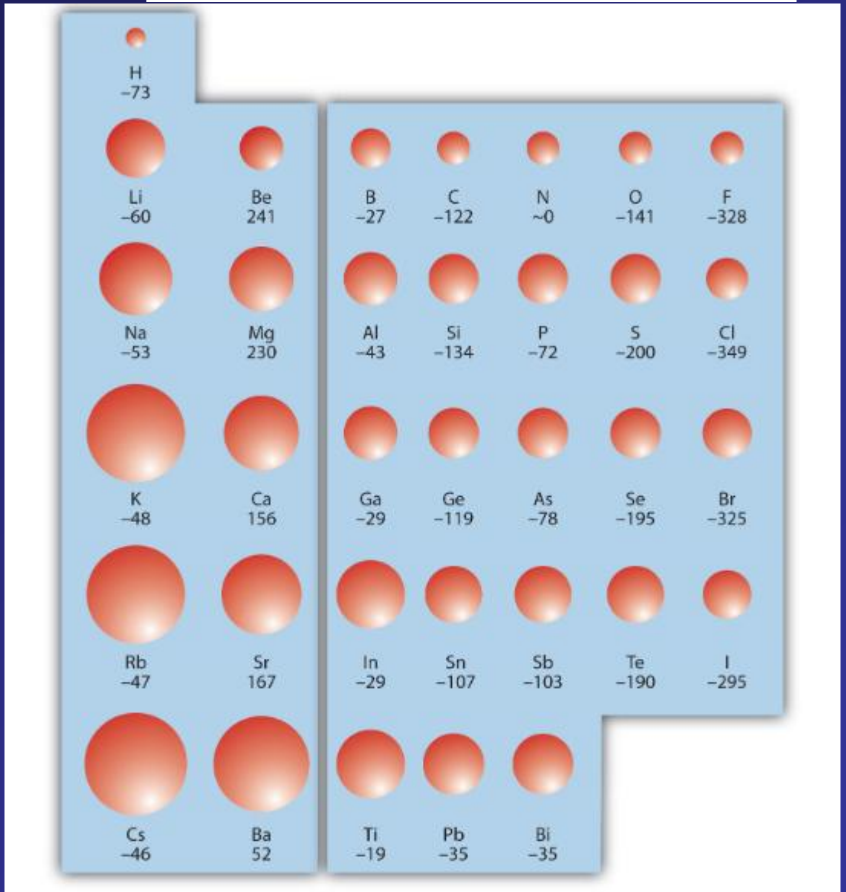
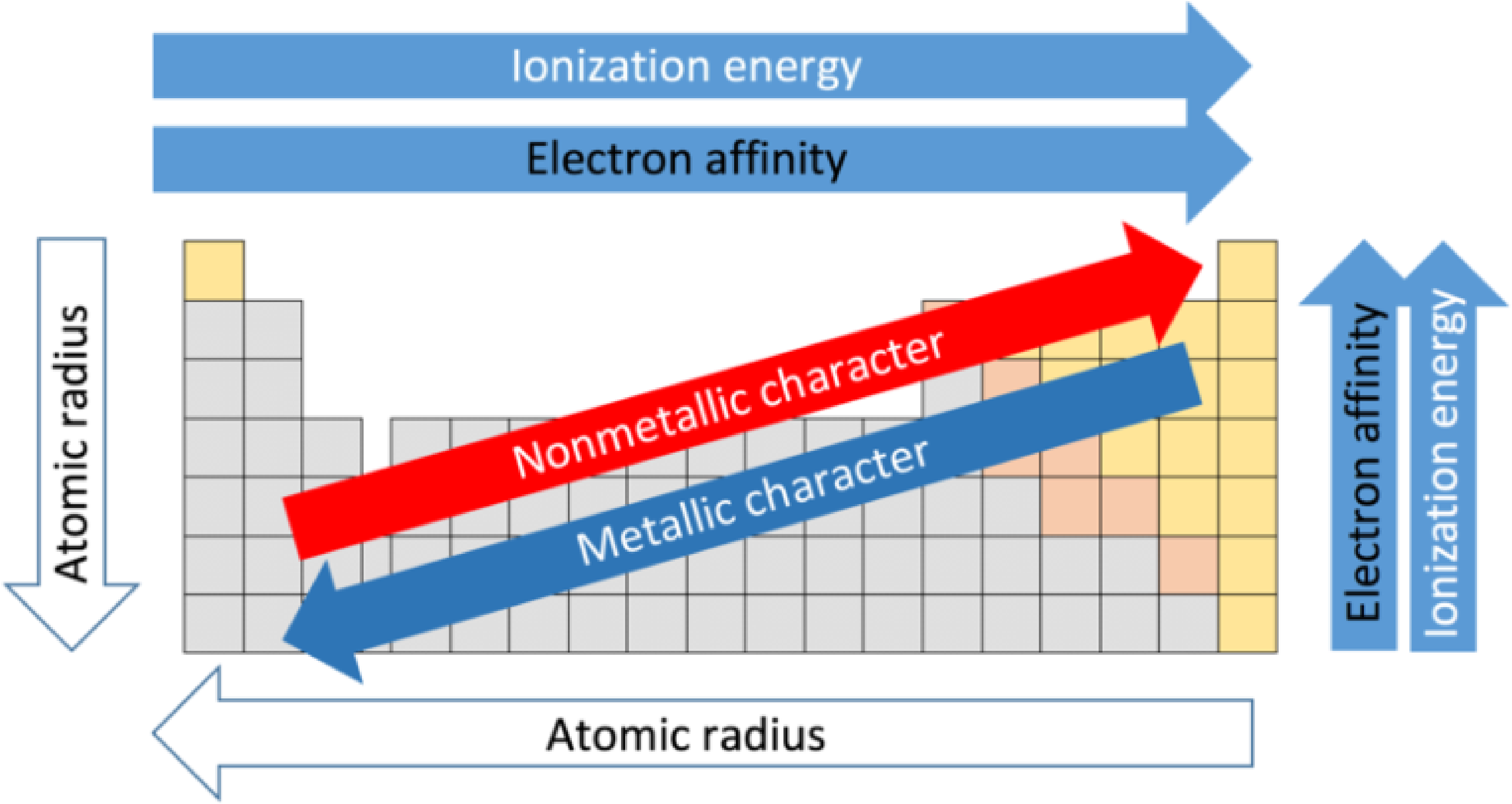


Figure 3.6.3: Electron Affinity on the Periodic Table. Values are in kJ/mol.

Summary of Periodic Trends



Various periodic trends (CC BY-SA 4.0; Sandbh via Wikipedia)