Scientific Discourse

Chemistry Series

3-Atomic Orbitals

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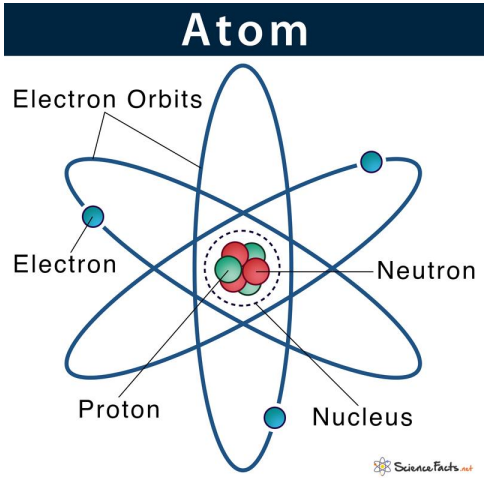
Slide 1

RECAP

So far, the hero of our story has discovered that:

- Chemistry is the study of how new substance(s) is/are formed from old substance(s)
  - A substance is a molecule.
  - A substance is something that is made up of two or more atoms.

- The solar system model of the atom
  - Protons
    - Positively charged particles
    - Concentrated in the nucleus
    - The Sun
  - Electrons
    - Negatively charged particles
    - Surround the nucleus.
    - The Planets



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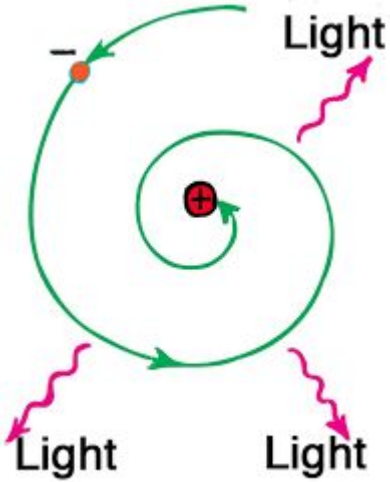
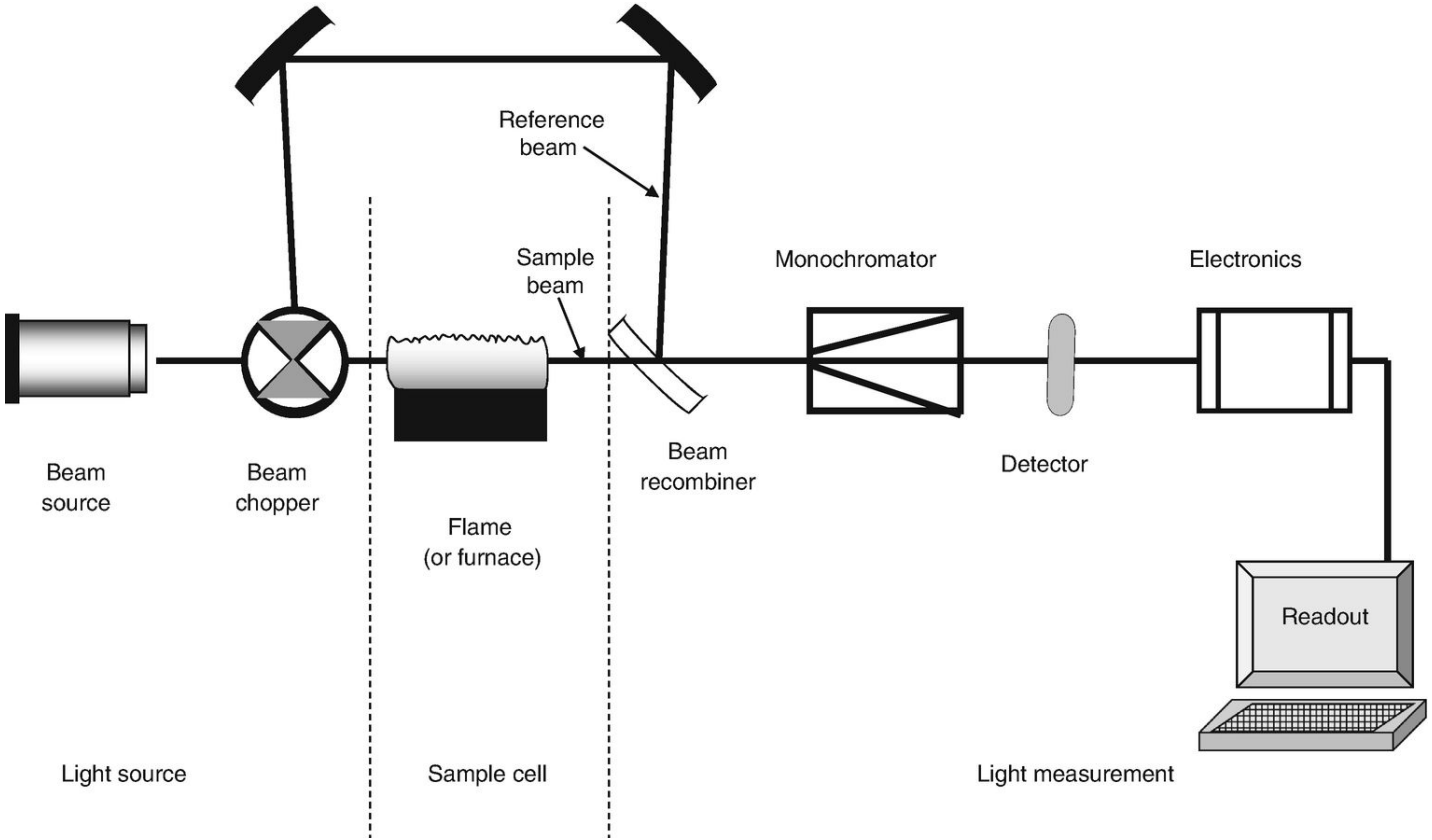
Why doesn’t the electron spiral into the nucleus?



Slide 3 Atomic Absorption Spectroscopy



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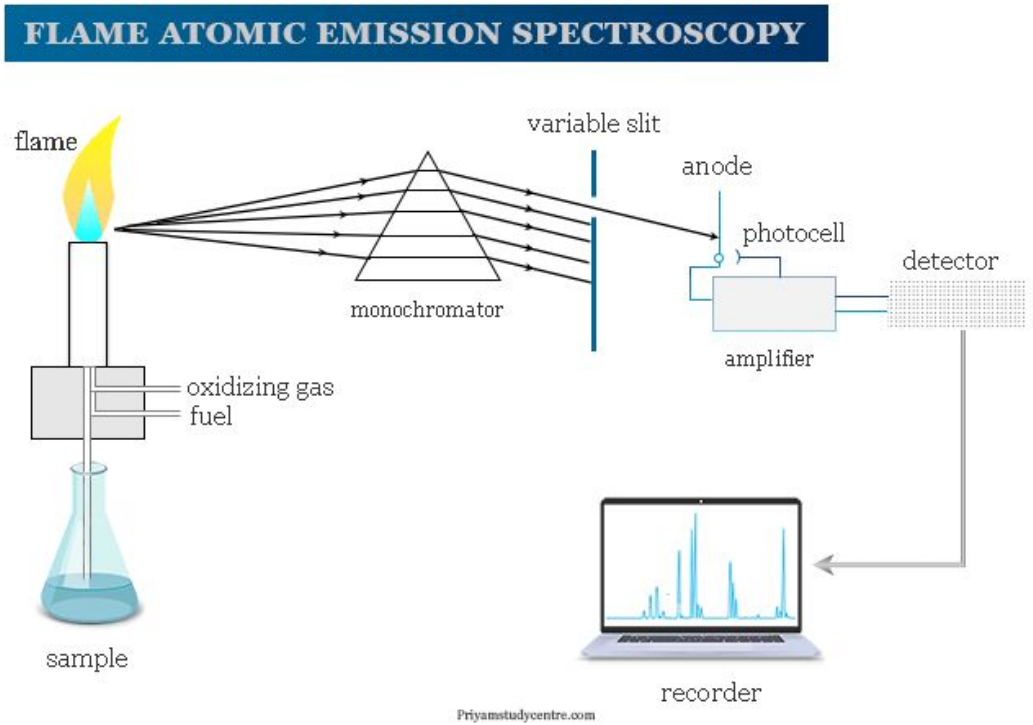
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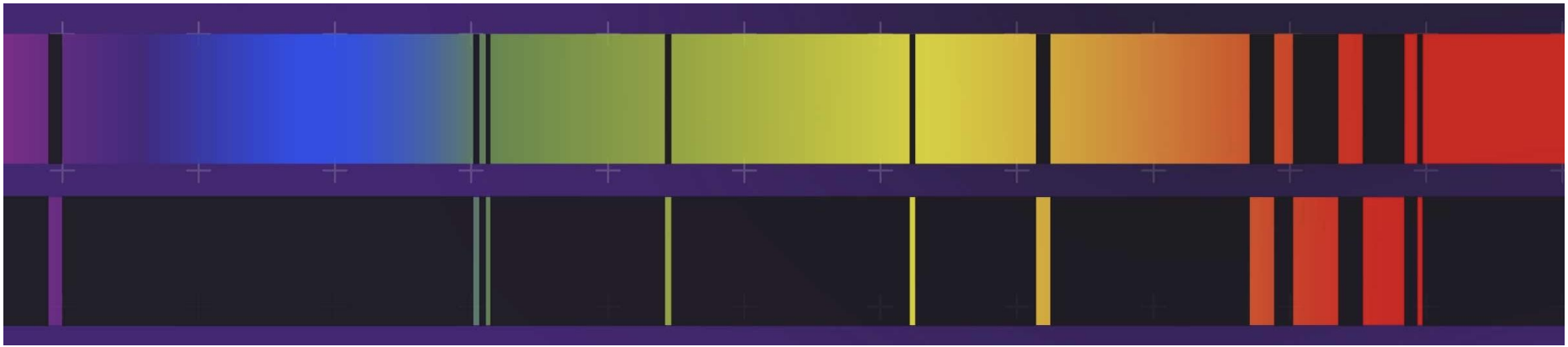

Spectrum of Neon

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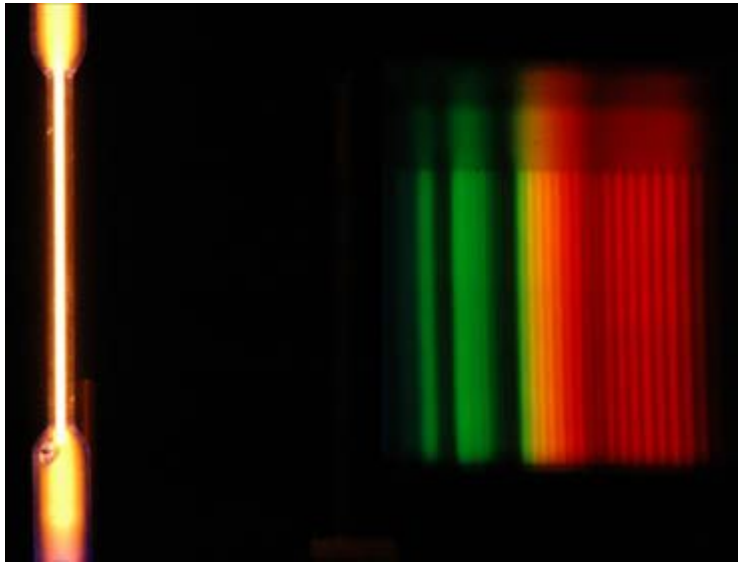

Spectrum of Nitrogen

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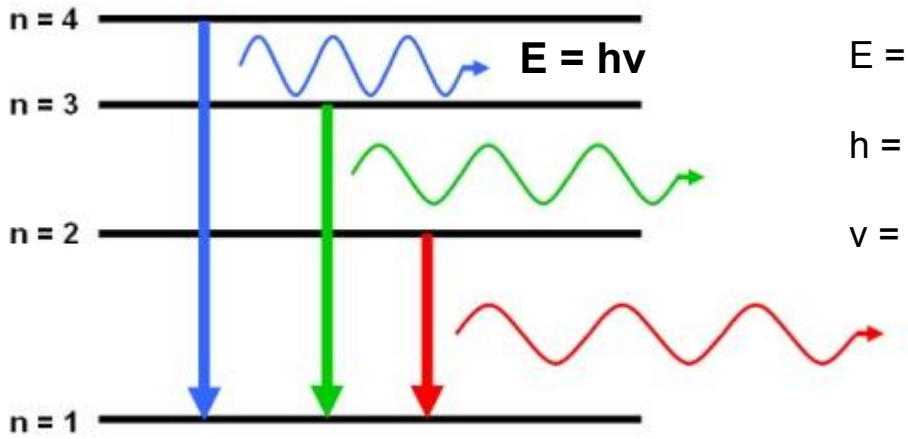


E = energy m^2 kg s^{-2} = joule

h = Planck's constant = 6.6×10^{-34} m^2 kg s^{-1}

v = (nu) light frequency s^{-1}

- hv is a discrete packet of energy.
- Each packet of energy has a discrete quantity of energy.
- A discrete quantity of something is a quantum of that thing.
- Hence, quantum mechanics.

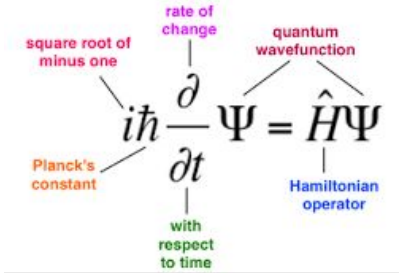
Schrodinger's Equation

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\mathrm{r}) + V(r)\Psi(\mathrm{r}) = E\Psi(\mathrm{r})$$

Basic Form

Kinetic Energy + *Potential Energy* = *Total Energy*

Time-Dependent Simplification



Time-Independent Simplification

$$\hat{H}\Psi = E\Psi$$

Hamiltonian Operator (Energy operator)

Energy eigenvalue

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- Schrodinger's equation is solved for psi (Ψ).
- Psi (Ψ) is a function of both time and space.
- It determines the shape of the wave function at any point in time and at any point in space.
- The shape of the wave function is related to the probability of the wave function existing at any point of time and at any point in space.
- The wave function is the same thing as the electron.

Orbital: space where the probability of finding the wave function (i.e., the electron) is ≥50%.

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- We can think of an orbital from different perspectives:
  - The energy level of an electron
  - The spatial position of the electron cloud
  - The probability of finding an electron

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- Shell: Collection of nearby energy states.
  - So far we have 7 shells

- Orbital: Energy states within each shell.
  -
  - There are four orbital types: s, p, d, and f

  - Note: Mathematically we can have additional orbitals in case a lot more elements are discovered.

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Shell	Orbital Types
1	s
2	s, p
3	s, p, d
4	s, p, d, f
5-7	s, p, d, f, ?

Orbital Type	Number of Orbital	Number of Electrons
s	1	2
p	3	6
d	5	10
f	7	14

Maximum of TWO electrons per each orbital.
Hund's Rule.

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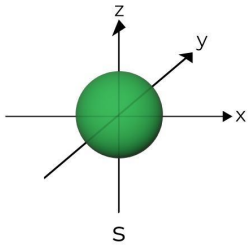
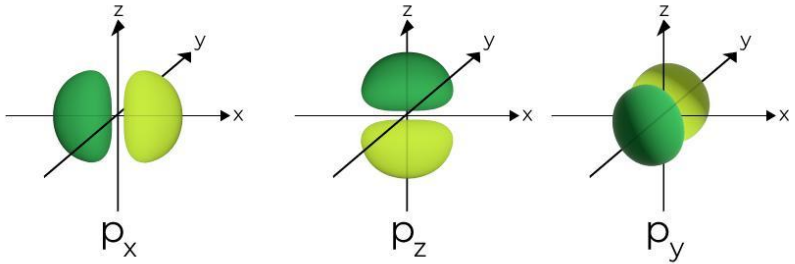
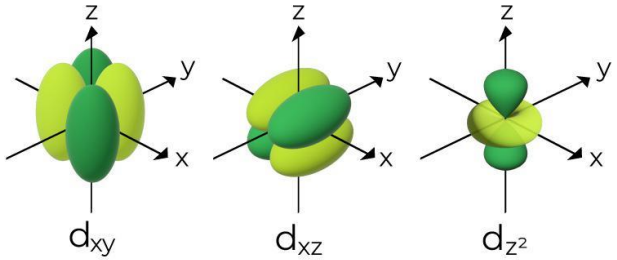


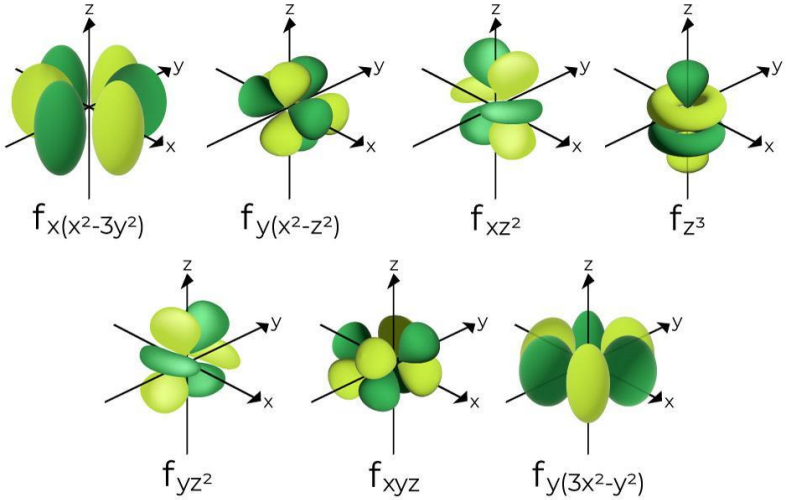
Shape of s-orbital



Shape of p-orbital



Shape of d-orbital



Shape of f-orbital

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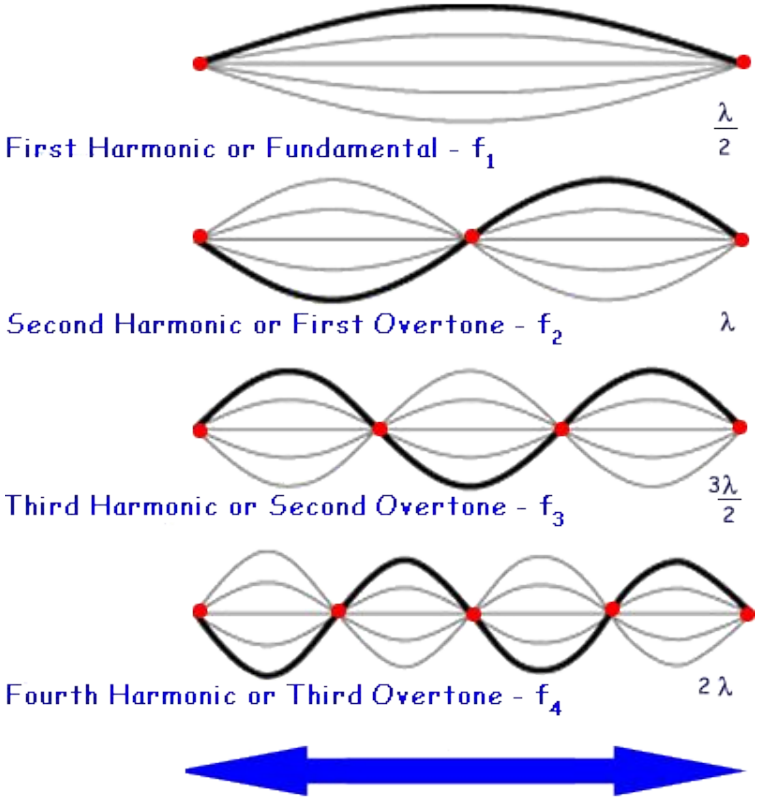
First Harmonic or Fundamental - f_1
$\frac{\lambda}{2}$
Second Harmonic or First Overtone - f_2
λ
Third Harmonic or Second Overtone - f_3
$\frac{3\lambda}{2}$
Fourth Harmonic or Third Overtone - f_4
2λ

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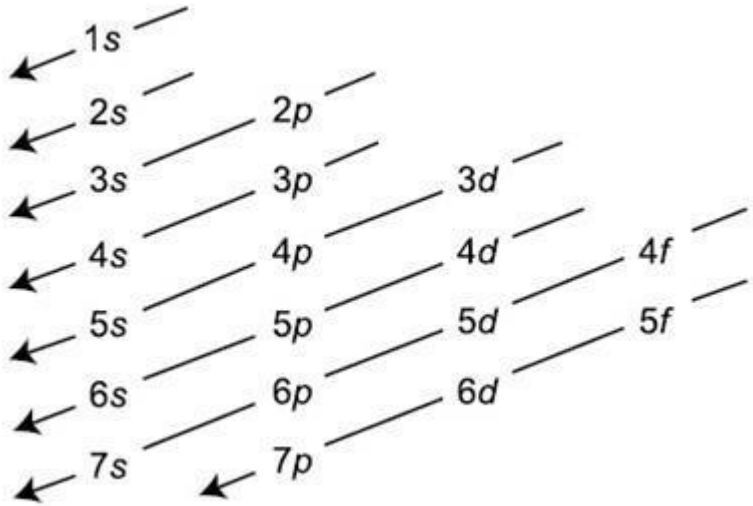

The Aufbau Principle: Gives us the relative energies of orbitals in a hydrogenic shell model (single proton, single atom, gas phase, in vacuum).

- Flawed. Fails for d and f block elements.
- Only works well for hydrogen.
- It has been significantly modified since the introduction of supercomputers.
    - Originally developed by Bohr and Pauli using a slide rule!
- Still used as a teaching tool.

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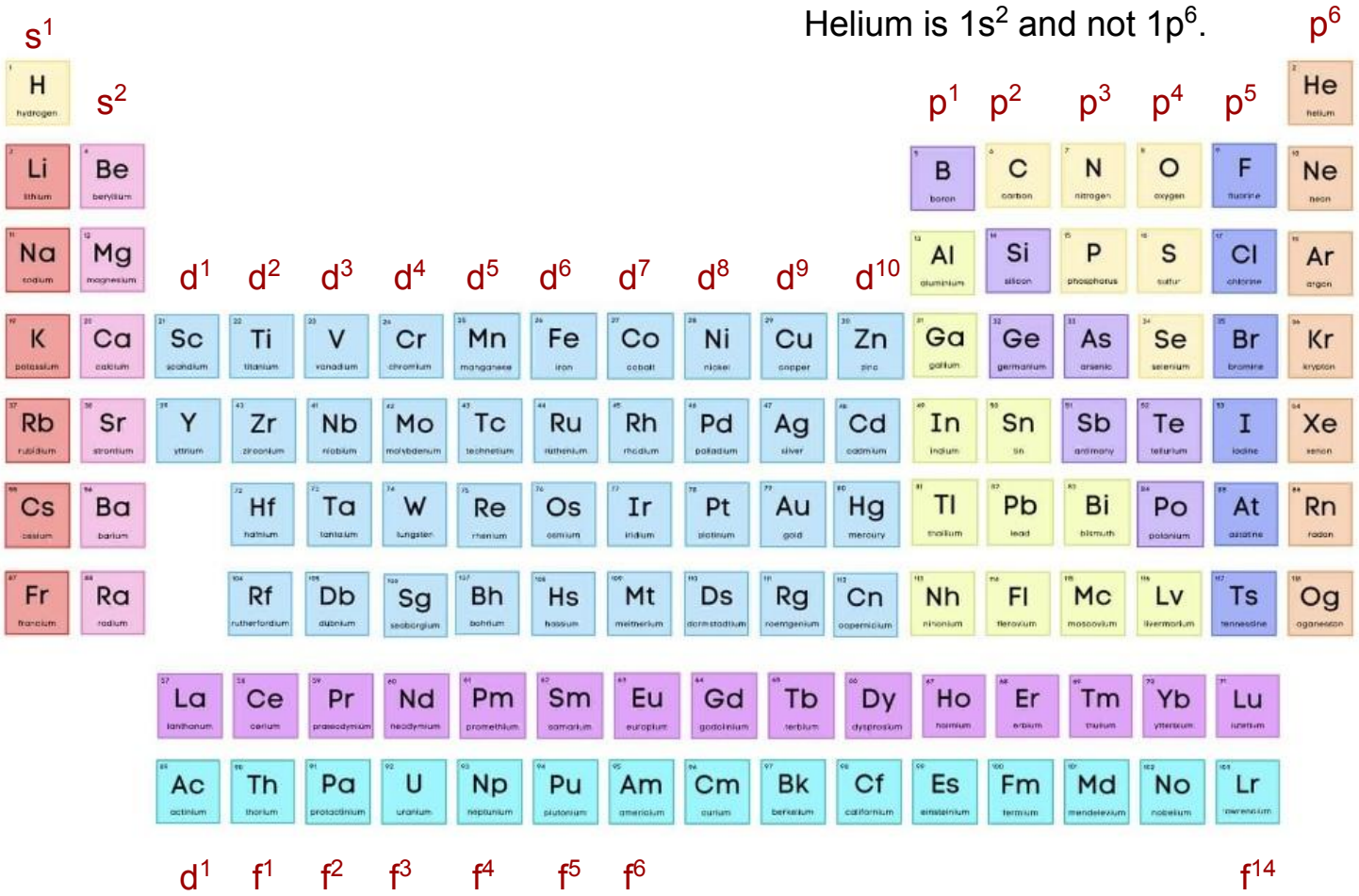
Helium is $1s^2$ and not $1p^6$.



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Take away lessons:

- The shapes of orbitals are graphic representation of the 50% probability space for finding electrons.
- Chemists approximate that electrons are clouds represented by orbitals.
- Different orbitals have different energy levels.
- Each orbital can have a maximum of two electrons.

Next time:

- The Octet Rule
- Hybridization
- Molecular orbitals
- Molecular geometry