Electron configuration of the Atom

where are the electrons?

Ⓐ **Bohr Model**: the condition of the electron in the early 1900's was based the following reasons.

1) Einstein and the photoelectric effect.

Einstein proposed that light energy was in the form of packets - "a shower of particles (photons) with energy equal to $h\nu$.

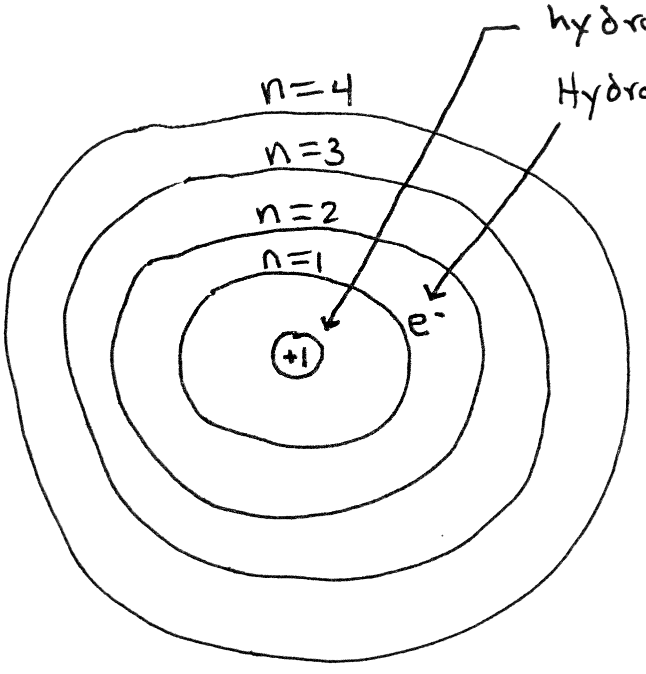
h = planck's constant
ν = frequency

It was observed that when certain metals were exposed to light of defined energy, electrons were dislodged. The effect was specific to the type of metal and the specific energy of the light.

2) when metal salts (eg. $NaCl$, $Ba(NO_3)_2$) were exposed to an energy source like a flame, light was produced. The light produced was a specific color and energy. The light produced is due to the movement of electrons between specific energy states or levels.

Bohr explained #1 and #2 by stating that the electron travels around the nucleus in discreet orbits with specific energies.

Bohr Model Hydrogen (1913)



hydrogen's proton where charge is +1

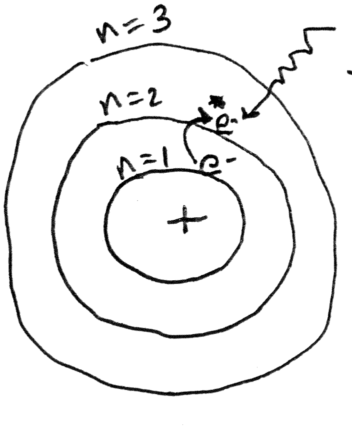
Hydrogen electron in energy level n = 1. Most stable = ground state

Bohr

- the e^- can only exist in n = 1, 2, 3, 4 . . . energy levels.
- The e^- cannot exist between energy levels.
- To move the e^- from n = 1 into higher energy levels, the exact energy difference between two energy levels must be absorbed by the atom.

- when an e^- is elevated to a higher energy level, the e^- and therefore the atom is at higher potential energy and is said to be in an excited state.

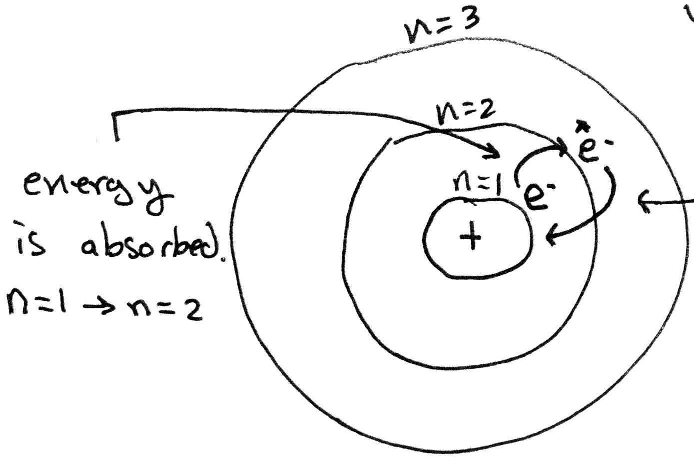
Excited State: An electron that has been elevated into a higher energy level due to absorption of energy.



Energy = can be light, heat, mechanical

The $^*e^-$ is in an excited state. The atom is in an excited state. The $^*e^-$ will not remain this way and will drop to a lower energy level. When the $^*e^-$ drops it gives off the energy difference in the form of light: where $\underset{\uparrow \text{energy}}{E} = \overset{\text{Planck's constant}}{h}\nu \leftarrow \text{frequency light}$

Energy is released as light when the e^- drops back to a lower energy level.



$n=2 \rightarrow n=1$: energy is released as light where

$E = h\nu$ ← planck's constant (h)

↑ energy (E) ↑ frequency of light (ν)

$E = h\nu$ and $\nu = \frac{c}{\lambda}$

frequency ↓ (ν)

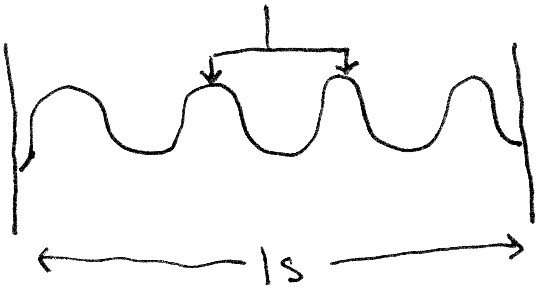
← speed of light (c)

← wavelength (λ)

Diagram to help you understand light.

Light wave

This distance is the wavelength = λ



ν = frequency = 4 peaks in one second so ν = 4 Hz

Hz = peaks per second

c = speed of light = constant and about 3×10^8 m/s

Light waves have energy (E) where

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

← speed of light (c)

← wavelength (λ)

↑ energy (E) ↑

The Bohr Model
Hydrogen Atom

- The electron has defined energy.
- The electron can be in energy level $n = 1, 2, 3, \ldots$
- The ground state is the lowest energy of the atom. The ground state is energy level 1.
- Energy must be absorbed to move from lower energy levels to higher energy levels. Energy is given off moving down energy levels.
- The energy released, is given off as light. The light is released as a line spectrum.

Beyond the Bohr Model

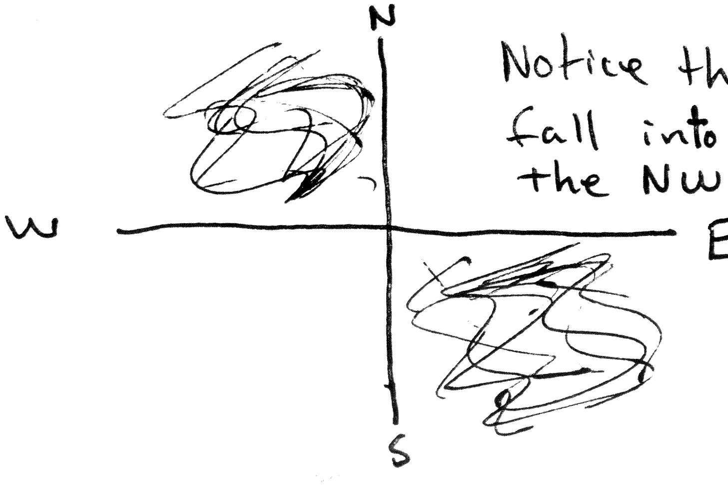
The Bohr model tells us that electrons have specific energies and that electrons can only exist in specific energy levels. The energy of the electron is lowest when it is closest to the proton(s).

Questions remain: where are the electrons? what is the electronic structure of the atom?

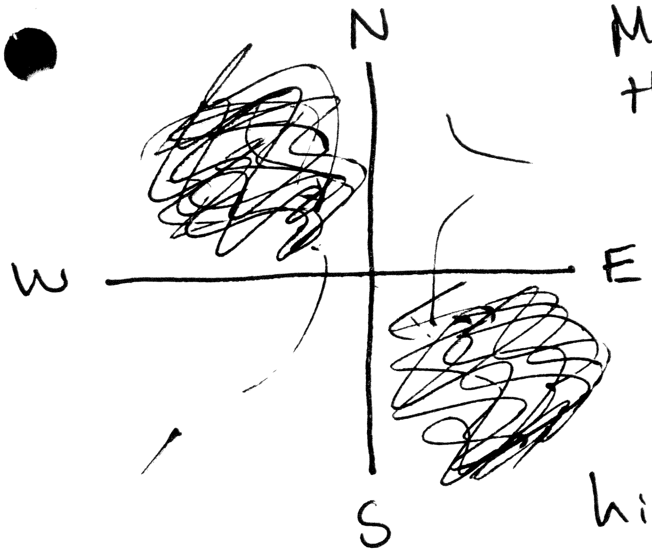
The main thing to understand at the beginning of this is that electrons do not have physical locations like humans do. We (humans) are massive objects by comparison to an electron and we move really slow. As I write this I am sitting in my study at home. I am in a fixed location. This is not how it is with electrons. Electrons are really small and they are moving really fast. A guy named Werner Heisenberg said that we cannot know precisely the position and the momentum of the electron.

One of the key principles about this is realizing that the electron has both particle and wave properties. So how can we describe electron structure?

If we can't know the location of the e⁻, how do we figure out where it is and what its characteristics are? To describe this we are going to pretend that I am an electron. I am going to attach a GPS to the top of my head and we are going to collect information about where I travel around Phoenix for the next 30 days (for pretend). After 1 month the data describing my travels is overlaid onto a map of Phoenix:

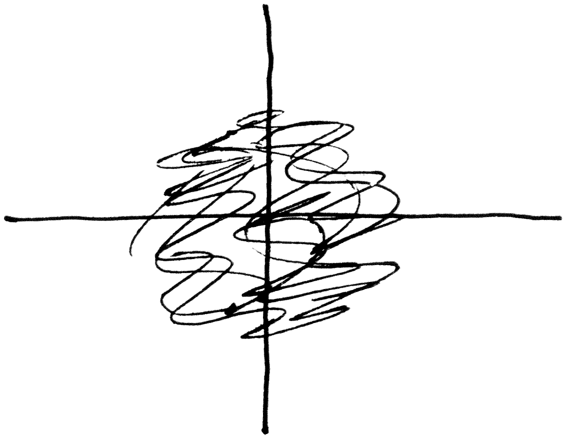


Notice that the tracings fall into two quadrants - the NW and SE parts of Phoenix.



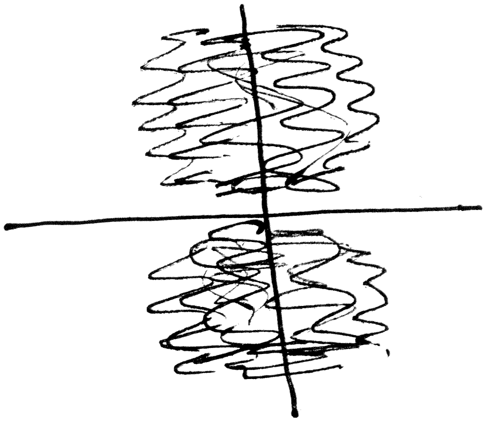
Most of my travels are in the NW and SE because I live in the NW (for pretend!) and work in the SE. The tracings represent a probability function. The highest probability of finding me is to look in the NW and SE part of the map. It wouldn't make sense to search for me in the SW or NE quadrants since I don't spend time in those areas. But common sense should prevail here meaning that if you find yourself on Chandler Blvd. the chances of seeing me are slim to none. The tracings represent a density map. The tracings also have an orientation - the shape is (∞) like a bar-bell or a lobe shape. Electron clouds are similar to the density map or probability function shown above.

Electron clouds or electron orbitals have tracings of two basic types:



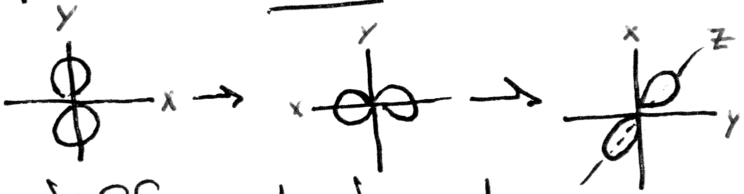
Spherical

and



lobed

The spherical orbitals are centered around the protons and do not have an orientation. The lobed orbitals also bracket or are centered around the protons and lobes have orientation.



The lobes can point in different directions.

The electron has 4 characteristics as defined by the Quantum Mechanical Model (QMM) of the atom (shrödinger).

QMM

The QMM Model provides four characteristics of the e^- called quantum numbers. So each e^- is characterised by 4 quantum numbers.

The characteristics are:

n = energy where $n = 1, 2, 3, \ldots$

l = Shape of orbital

m_l = orientation of orbital

m_s = spin of e^-

n number

The n number defines the energy of the e^- and is the same as Bohr's n number. So $n=1$ is the energy level closest to the protons. $n=7$ is farthest from the protons.

l number

Orbitals have essentially two kinds of shapes: Spherical and lobed. The Spherical orbitals are called "s" orbitals and each energy level has one s orbital. An s orbital holds a maximum of $2e^-$.

The lobed orbitals are comprised of 3 types: P, d, f. The P system has 3 suborbitals where each suborbital holds $2e^-$. So the P system will hold a max. of $6e^-$. The d system has 5 suborbitals and holds a max of $10e^-$. The f has 7 suborbitals and holds a max of $14e^-$. Putting all of this together the basic electron Structure of the atom is:

1S 2S2P 3S3P 4S 3d4P...

Protons $\underset{1}{\underline{1S}}\ \ \underset{2}{\underline{2S2P}}\ \ \underset{3}{\underline{3S3P}}\ \underset{4}{\underline{4S3d4P\ldots}}$

I have underlined each major energy level. you can see that each energy level has an "S" orbital. Starting with $n=2$, each energy level has a "P" system. In $n=3$ the "d" system appears. The electron structure shown above takes care of elements from H to Kr. We follow the Auf Bau principle when filling the electron configuration (EC) which states that we fill from $n=1$ moving up in energy. For $\overset{1}{H}$ the EC is $1S^1$. For $\overset{2}{He}$ the EC is $1S^2$.

$\overset{1}{H}\ 1S^1$ ↖ H's single e^-

$\overset{2}{He}\ 1S^2$ ↖ He's 2 e^-.

For $\overset{3}{Li}$ the EC is $1S^2 2S^1$. $\overset{4}{Be}$ is $1S^2 2S^2$ and so on.

Electron Configuration

A method to order the electrons for any given atom from lowest energy (closest to the nucleus) to highest energy (farthest from the nucleus).

The basic Scheme:

1S 2S2P 3S3P 4S 3d 4P

Number: is energy level; 1, 2, 3 - - - where 1 is lowest energy.

letter: orbital

S = holds 2e⁻

P = holds 6e⁻

d = holds 10e⁻

Fill starting with the 1S. When 2e⁻ are in 1S move up to the 2S, then to the 2P and so on.

Example

$\overset{3}{\mathrm{Li}}$ - neutral Li has 3e⁻ so $1S^2 2S^1$; place 2e⁻ in 1S and 1e⁻ in the 2S.

$\overset{5}{\mathrm{B}}$ $1S^2 2S^2 2p^1$

$\overset{7}{\mathrm{N}}$ $1S^2 2S^2 2p^3$

$\overset{8}{\mathrm{O}}$ $1S^2 2S^2 2p^4$

$\overset{11}{\mathrm{Na}}$ $1S^2 2S^2 2p^6 3S^1$

Purpose of Electron Configuration (EC):

EC allows you to identify the electron structure and the number of electrons in the outermost energy level (valence) of any given atom. This is important because the outermost electrons determine the reactivity of a particular element. For example, if we look at the outer most electrons (valence) of the atoms in several groups we can see trends:

1A

H $1s^1$
Li $2s^1$
Na $3s^1$
K $4s^1$
Rb $5s^1$
Cs $6s^1$

2A

Be $2S^2$
Mg $3S^2$
Ca $4S^2$
Sr $5S^2$
Ba $6S^2$

5A

N $2s^2 2p^3$
P $3s^2 3p^3$

6A

O $2s^2 2p^4$
S $3s^2 3p^4$

7A

F $2s^2 2p^5$
Cl $3s^2 3p^5$
Br $4s^2 4p^5$
I $5s^2 5p^5$

8A

He $1s^2$
Ne $2s^2 2p^6$
Ar $3s^2 3p^6$

All elements in 8A have full outer energy levels. This is why they are unreactive.

Orbital Diagrams (OD): An OD provides a method to observe all four quantum numbers for a given <u>electron</u>. The OD is written using platforms or boxes and e^- are ~~[illegible]~~ represented with arrows, ↿ or ↑.

<u>Example</u>

$\overset{1}{H}$ $1s^1$ so $\underset{1s}{\underline{\ \upharpoonleft\ }}$ or $\underset{1s}{-\boxed{\upharpoonleft}-}$

<u>Notes</u>

1. Any single electron appearing in an orbital will have an up spin, ↿ or ↑.
2. Hunds Rule is followed. The lowest energy configuration is the one with the <u>most unpaired electrons</u>.
3. For suborbitals, place electrons in the left most platform first. Back fill only after all platforms have one e^-.
4. The above are <u>conventions</u> <u>only</u>. I'll come back to this issue later.

7. EC and OD

OD's Period 2 - note Hund's Rule: the lowest energy configuration for any atom is the one with the most unpaired e^-'s.

^{3}Li EC = $1S^2 2S^1$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow}}$

^{4}Be EC = $1S^2 2S^2$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}$

^{5}B EC = $1S^2 2S^2 2p^1$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow}\ \underline{\ \ }\ \underline{\ \ }}_{2P}$

^{6}C EC = $1S^2 2S^2 2p^2$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow}\ \underline{\uparrow}\ \underline{\ \ }}_{2P}$

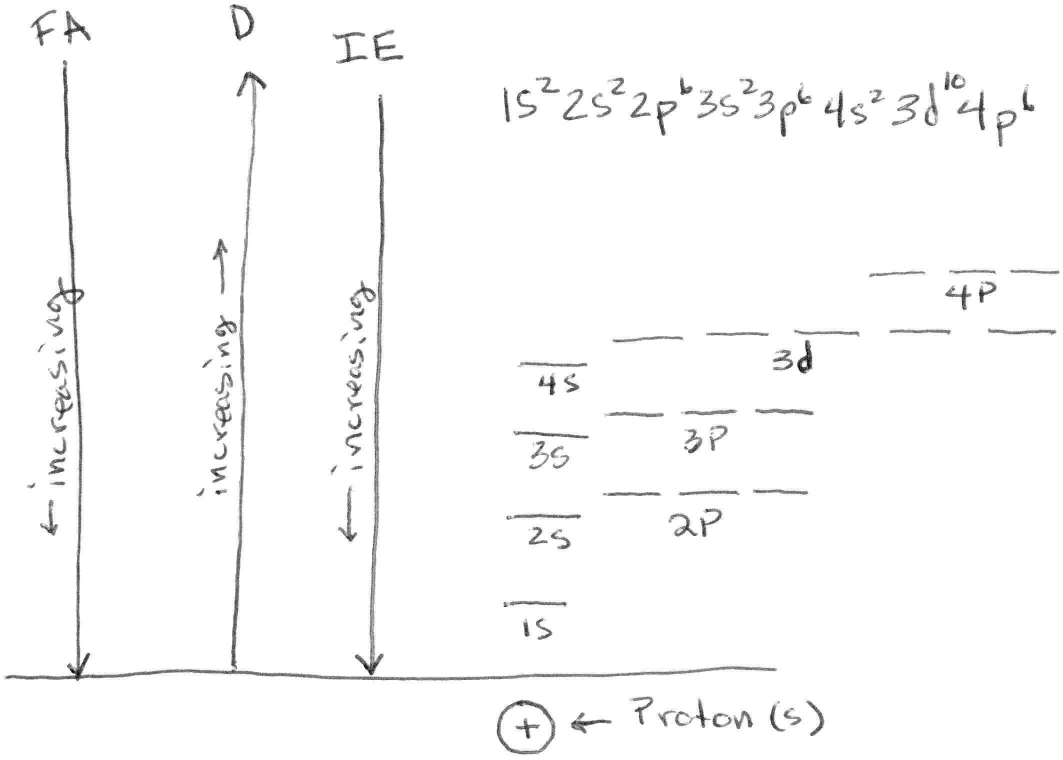
^{7}N EC = $1S^2 2S^2 2p^3$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow}\ \underline{\uparrow}\ \underline{\uparrow}}_{2P}$

^{8}O EC = $1S^2 2S^2 2p^4$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow\downarrow}\ \underline{\uparrow}\ \underline{\uparrow}}_{2P}$

^{9}F EC = $1S^2 2S^2 2p^5$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow}}_{2P}$

^{10}Ne EC = $1S^2 2S^2 2p^6$ OD = $\underset{1S}{\underline{\uparrow\downarrow}}\ \underset{2S}{\underline{\uparrow\downarrow}}\ \underbrace{\underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}\ \underline{\uparrow\downarrow}}_{2P}$

Electron Configuration and Energy of the electron, e^-.



$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

IE = ionization energy = the energy required to remove an e^-.

D = distance from proton(s)

FA = force of attraction = how hard the protons pull on the e^-.

This diagram accurately relates IE and FA for elements 1-20.

IE increases for e^- closer to the protons because FA is higher. Thus, its easier to remove an e^- from the 2s suborbital than the 1s orbital.

Valence Electrons versus Core Electrons

Valence electrons are important because they are the electrons involved in ALL bonding.

Valence Electrons: the e⁻ found in the outermost energy level of the atom.

Core Electrons: the electrons found in the energy levels preceding the valence electrons.

Examples

$${}^{3}\text{Li}\ \underbrace{\boxed{1s^2}}_{\text{core}}\underbrace{2s^1}_{\text{valence}} \qquad {}^{6}\text{C}\ \underbrace{\boxed{1s^2}}_{\text{core}}\underbrace{2s^2 2p^2}_{\text{valence}}$$

$${}^{11}\text{Na}\ \underbrace{\boxed{1s^2 2s^2 2p^6}}_{\text{core}}\underbrace{3s^1}_{\text{valence}} \qquad {}^{14}\text{Si}\ \underbrace{\boxed{1s^2 2s^2 2p^6}}_{\text{core}}\underbrace{3s^2 3p^2}_{\text{valence}}$$

The reactivity of an element is due to the valence electrons. Formation of bonds is a result of valence e⁻. Valence e⁻ also influence the physical properties of elements.