- Giving the four parameters will uniquely identify an electron around an atom. No two electrons in the same atom can share all four. These parameters are called QUANTUM NUMBERS.

(1) PRINCIPAL QUANTUM NUMBER (n):

- "energy level", "shell"
- Represents two things:
  * The distance of the electron from the nucleus.
  * Energy. "n" is one factor that contributes to the energy of the electron.

$n = 1, 2, 3, 4, \ldots$ (integers)

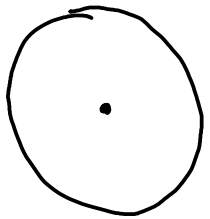
(2) ANGULAR MOMENTUM QUANTUM NUMBER: ℓ

- "subshell"
- Represents the SHAPE of the region of space where the electron is found.
  - (Bohr assumed CIRCULAR orbits for electrons ... but there are more possibilities.)

-"l" also contributes ENERGY. Higher values for "l" mean the electron has higher energy.

ℓ = 0 to n-1 , integers

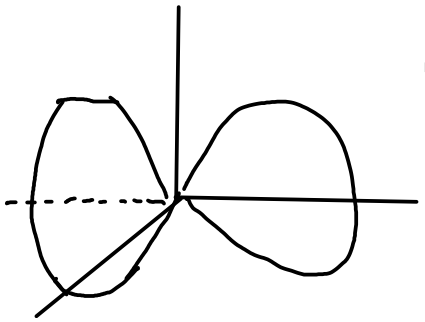
n = 1 ; ℓ = 0



"l" = 0 ; spherical subshell

Also called an "s" subshell.

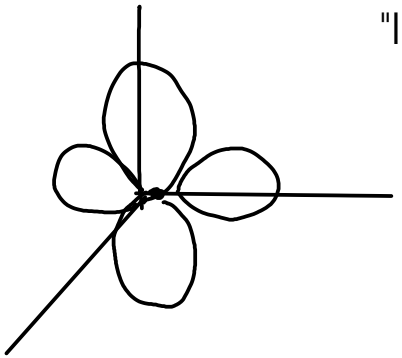
n = 2 ; ℓ = 0, 1



"l"=1 ; dumbbell shaped

Also called a "p" subshell

n = 3, ℓ = 0, 1, 2



"l"=2; flower-shaped

Also called a "d" subshell

(p 285, 3-D pictures of subshells)

Higher values for "l" translate to higher energies for the electron!

For convenience, and partially for historical reasons, we use letters to designate the different subshells. (p 290, 10th ed)

ℓ = 0 "s"

ℓ = 1 "p"

ℓ = 2 "d"

ℓ = 3 "f"

ℓ = 4 "g"

↓ The rest follow the alphabet

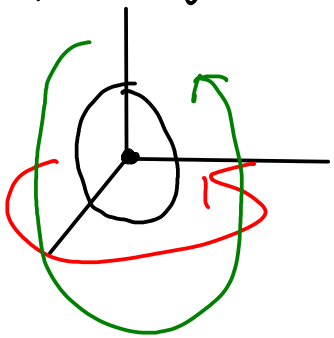
(3) MAGNETIC QUANTUM NUMBER m_ℓ

- Represents the ORIENTATION of a subshell in 3D space.

$m_\ell = -\ell$ to $+\ell$, integers

$\ell = 0$, $m_\ell = 0$

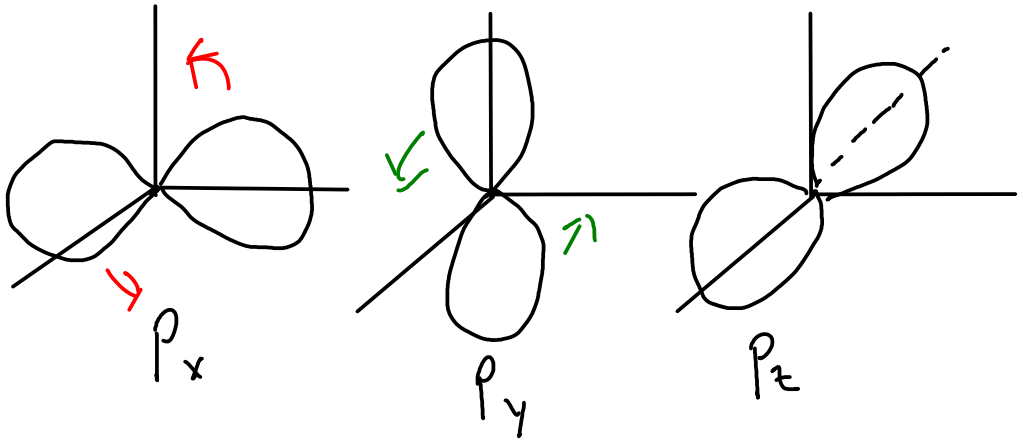
"s"



There is only one possible orientation for an "s" subshell!

$\ell = 1$; $m_\ell = -1, 0, 1$

"p"



There are THREE possible orientations for a "p" subshell!

$\ell = 2$, $m_\ell = -2, -1, 0, 1, 2$ (five orentations)

"d"

picture p285, p290 (tenth)

$\ell = 3$, $m_\ell = -3, -2, -1, 0, 1, 2, 3$ (seven orentations)

"f"

... all the arrangements of a single subshell have the same energy. The magnetic quantum number DOESN'T contribute to the energy of an electron.

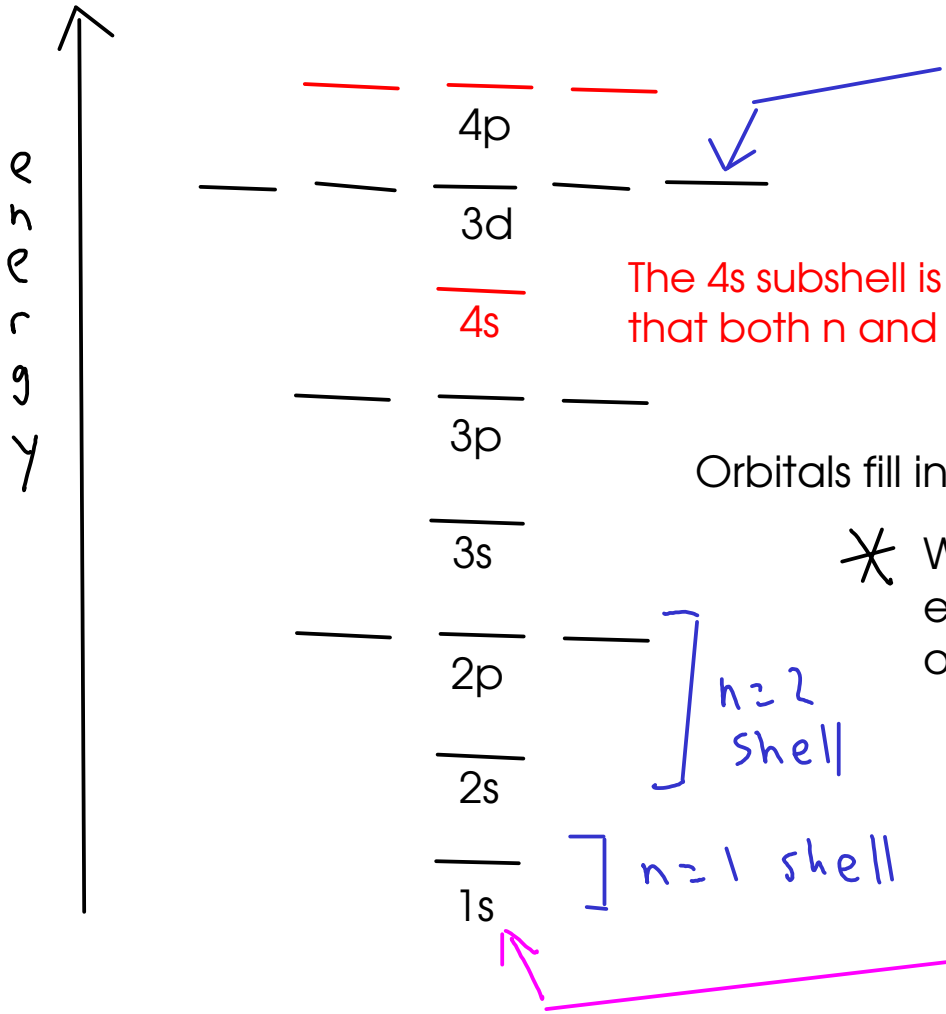
(4) (MAGNETIC) SPIN QUANTUM NUMBER: m_s

$m_s = -1/2$ OR $+1/2$ "spin down" or "spin up"

- An ORBITAL (region with fixed "n", "l" and "ml" values) can hold TWO electrons.

ORBITAL DIAGRAM

- A graphical representation of the quantum number "map" of electrons around an atom.



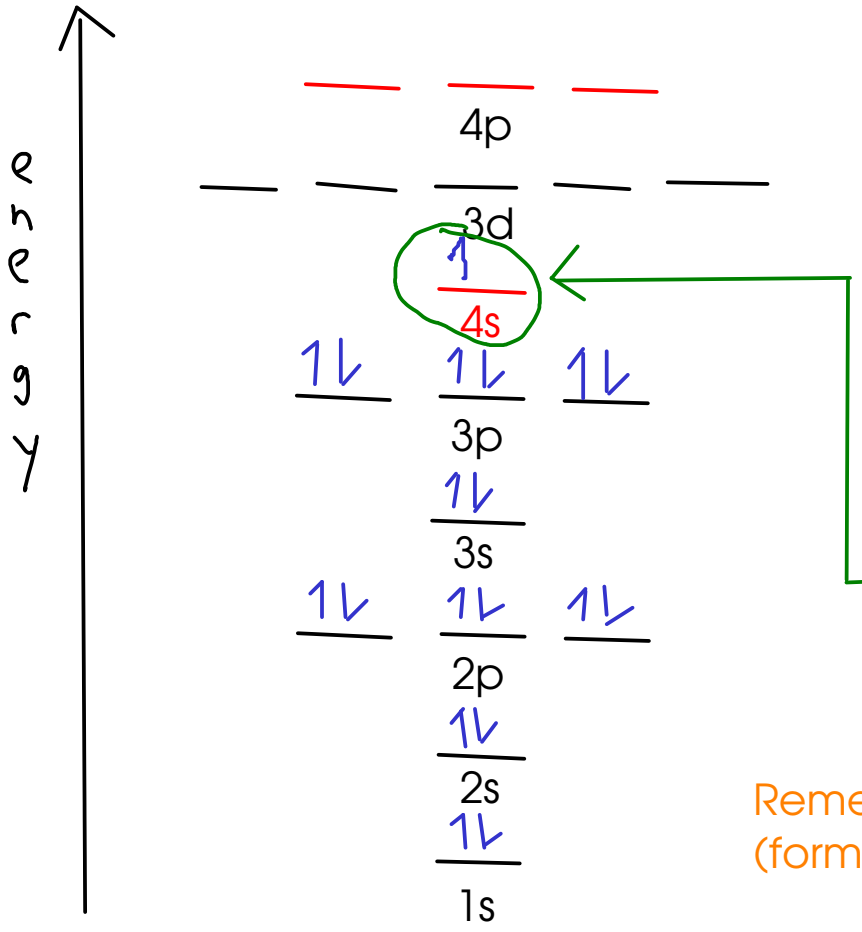
Each blank represents an ORBITAL, and can hold two electrons.

The 4s subshell is lower energy than the 3d subshells .... remember that both n and "l" contribute to energy!

Orbitals fill in order: The lower energy orbitals fill first.

* Where there's more than one orbital with the same energy, electrons don't pair up until each one has one electron in it!

1s: This means the first shell (n=1) and the "s" subshell ("l"=0)



How would an orbital diagram for the element POTASSIUM look?

K , Z = 19

└ atomic number

Electrons in the outermost shell of an atom are called VALENCE electrons. THESE electrons are normally involved in chemical bonding.

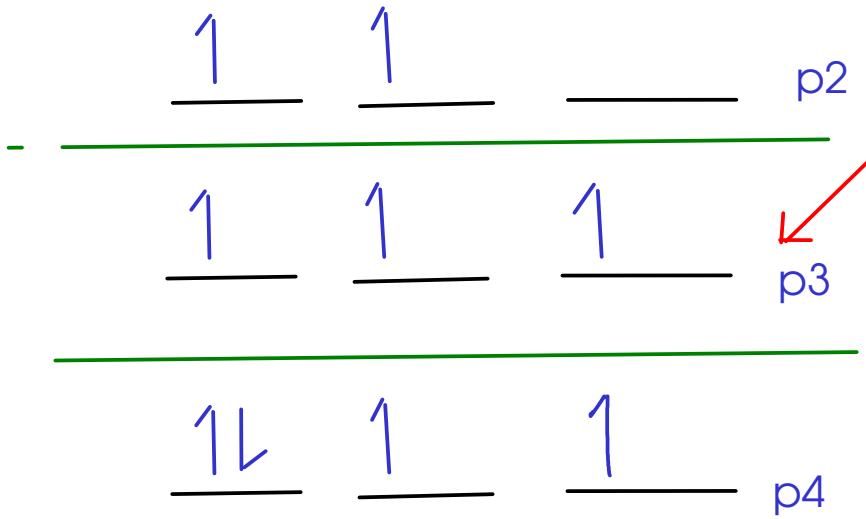
Remember: Potassium tends to lose a single electron (forming a cation) in chemical reactions. K^+

A note on chemical bonding and electron arrangement:

- Filled and half-filled subshells seem to be preferred by atoms.

Hund's Rule

- When you have two or more orbitals with equivalent energy, electrons will go into each equivalent orbital BEFORE pairing. Pairing costs a bit of energy - less than going to a higher-energy orbital, but more than going to another equivalent orbital.



Electron configurations with filled subshells OR HALF-FILLED SUBSHELLS are more stable than other configurations.
(can explain some transition metal chemistry)

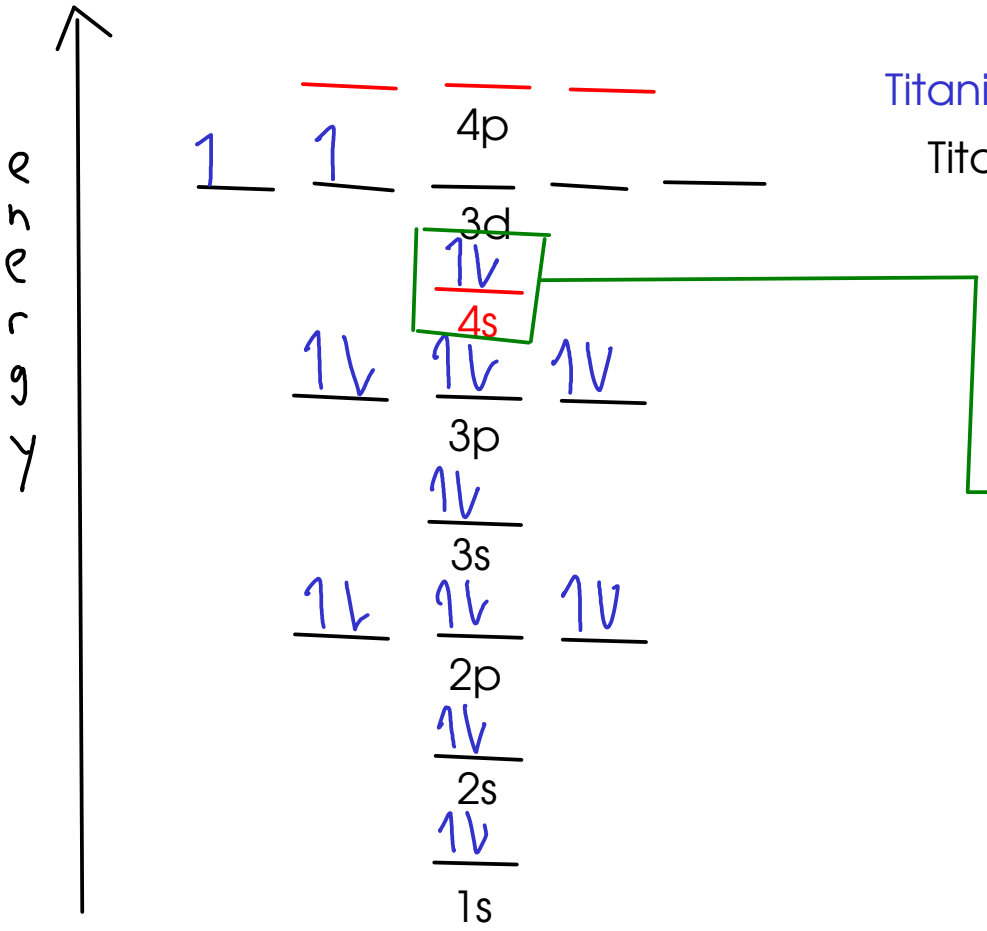
Electrons begin to pair only AFTER all equivalent "p" orbitals are full.

Experimental evidence for Hund's rule:

"Paramagnetism" - attraction of an atom to a magnetic field

* Spinning electrons are magnetic, but OPPOSITE spins cancel each other out.
* Atoms with unpaired electrons are paramagnetic, while atoms containing only paired electrons are not.

A little bit about transition metals...



Titanium (Ti, Z = 22)

Titanium usually forms one of two ions: +2 and +4

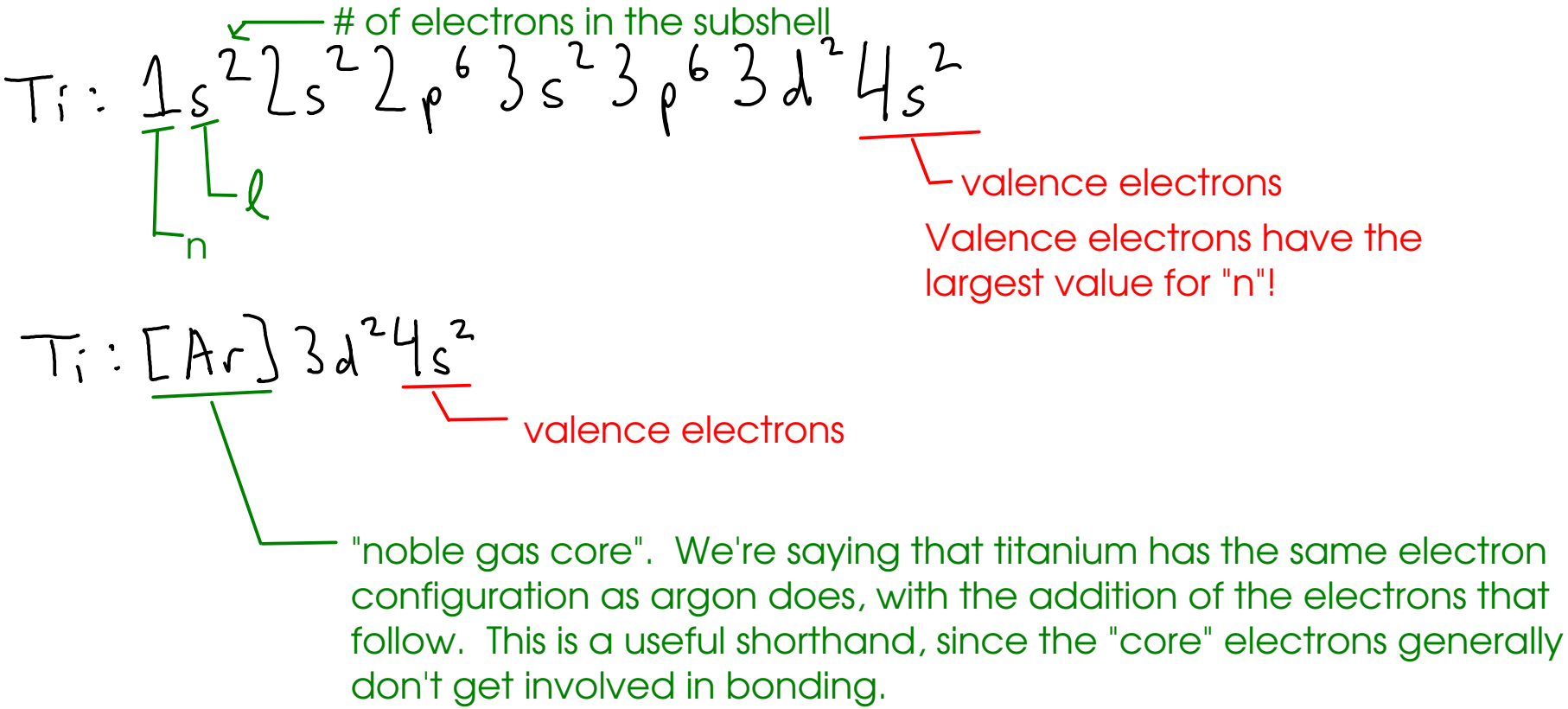
- if Ti loses only the valence electrons, forms +2. If it also loses the 3d electrons, forms +4.

valence electrons

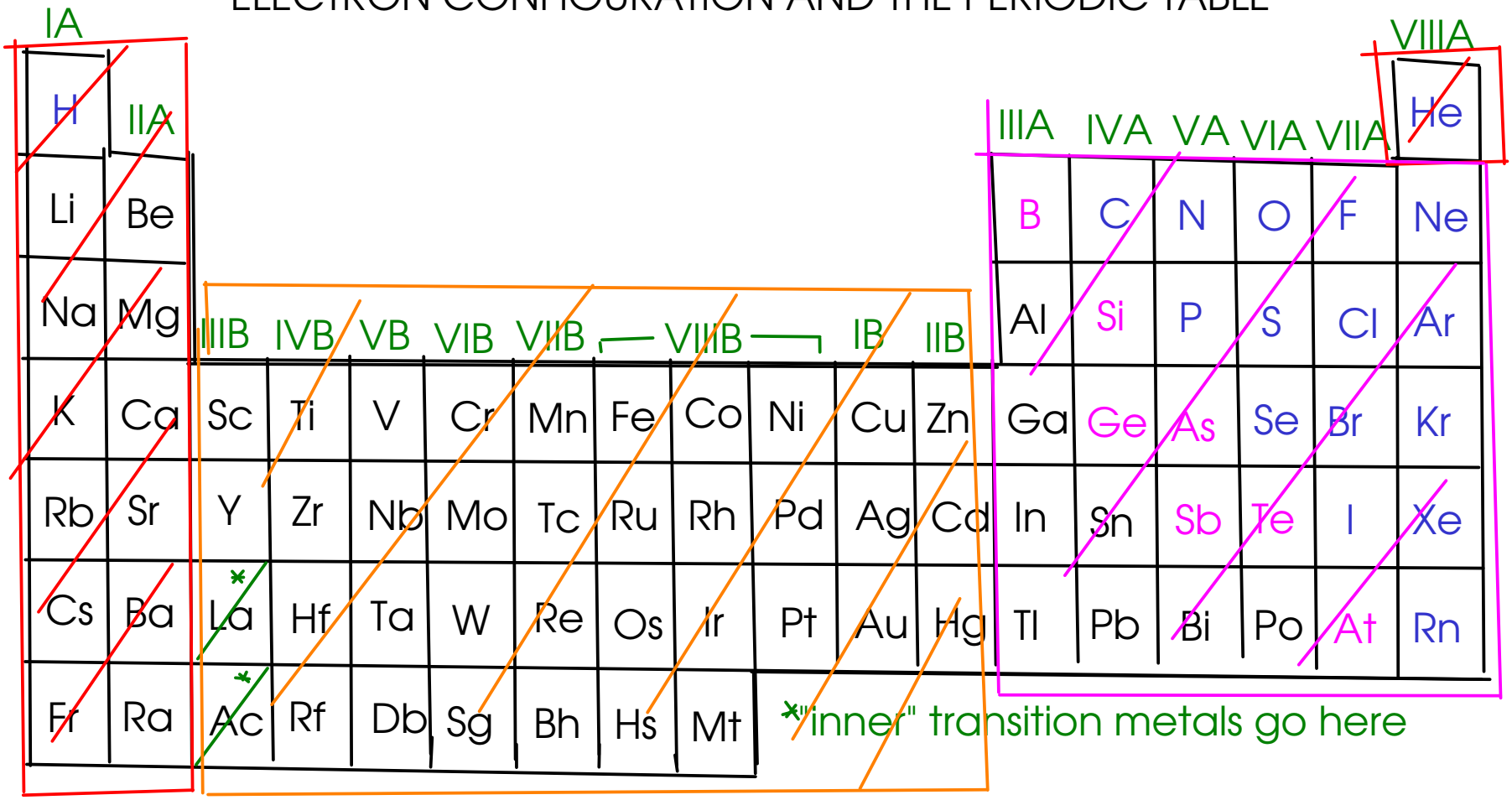
- Most transition metals have TWO valence electrons (in an "s" subshell), and the other ions they form come from electron loss in "d" subshells.

ELECTRON CONFIGURATION (SHORT FORM)

- We can represent the electron configuration without drawing a diagram or writing down pages of quantum numbers every time. We write the "electron configuration".



ELECTRON CONFIGURATION AND THE PERIODIC TABLE

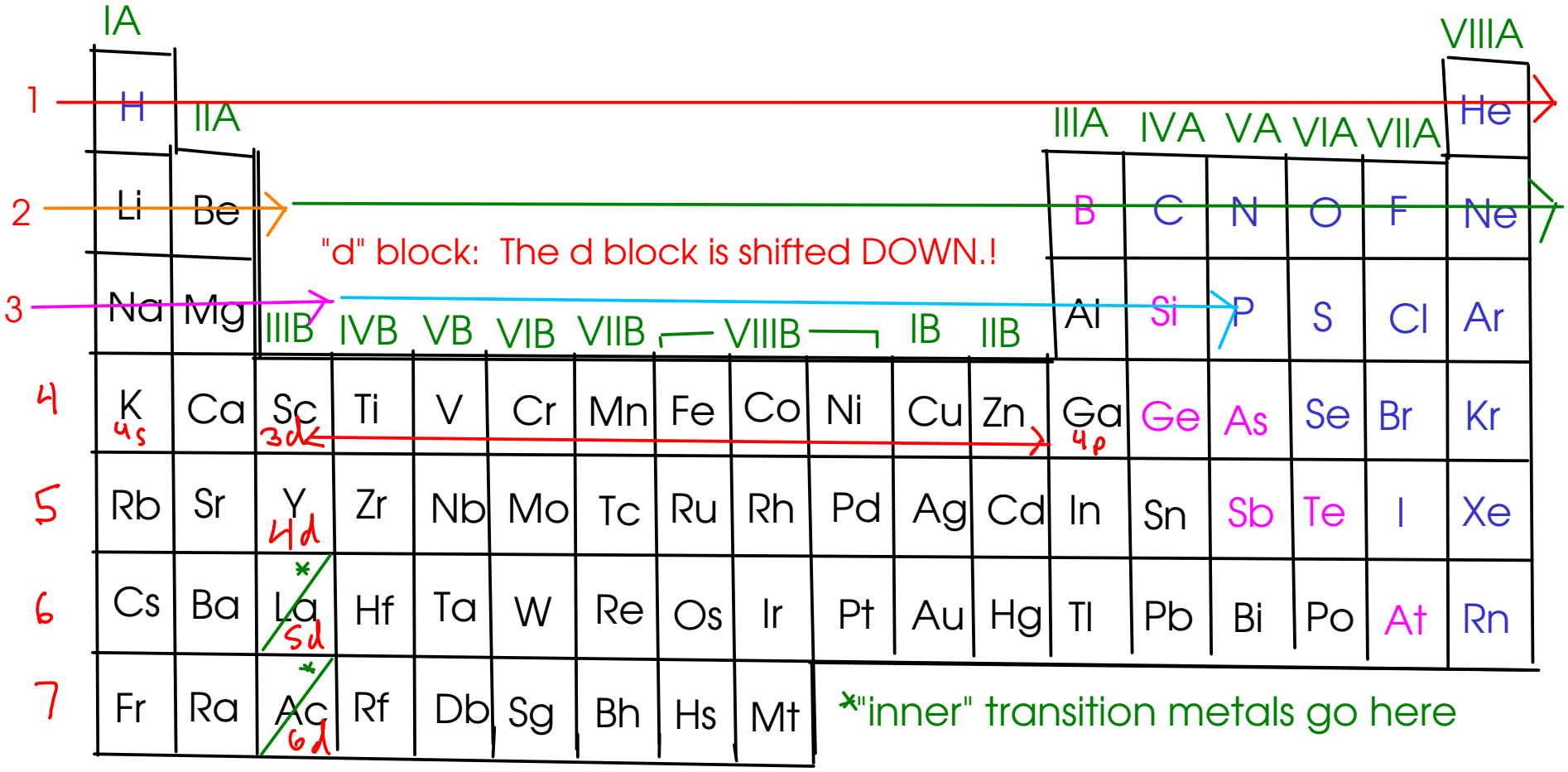


"s" block: last electron in these atoms is in an "s" orbital!

"p" block: last electron in these atoms is in a "p" orbital!

"d" block: last electron in these atoms is in a "d" orbital

- To write an electron configuration using the periodic table, start at hydrogen, and count up the electrons until you reach your element!



Example: Phosphorus (P): $1s^2 2s^2 2p^6 3s^2 3p^3$

Noble gas core notation for P: $[Ne]3s^2 3p^3$

EXAMPLES:

F $1s^2 2s^2 2p^5$

Remember - valence electrons are ALL of the electrons in the outermost SHELL (n)! More that one subshell (l) may be included in the valence electrons

S $1s^2 2s^2 2p^6 3s^2 3p^4$

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

$[Ne] 3s^2 3p^5$

TITANIUM is a transition metal that commonly forms either +2 or +4 cations. The 4s electrons are lost when the +2 ion forms, while the 4s AND 3d electrons are lost to form the +4!

You can order the subshells in numeric order OR in filling order

Ti $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$ or $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$

or $[Ar] 3d^2 4s^2$ or $[Ar] 4s^2 3d^2$

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

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

Noble gas core notation. Use the previous noble gas on the table, then add the electrons that it doesn't have to the end.

Kr $[Ar] 3d^{10} 4s^2 4p^6$

~~[Kr]~~

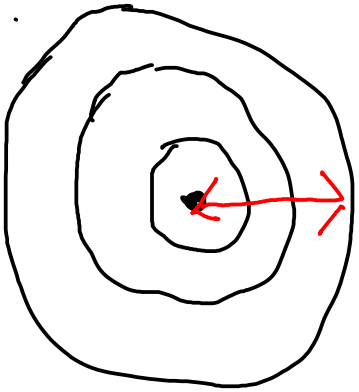
Sample f-block element

Ce: $[Xe] 6s^2 5d^1 4f^1$

PERIODIC TRENDS

- Some properties of elements can be related to their positions on the periodic table.

ATOMIC RADIUS



- The distance between the nucleus of the atoms and the outermost shell of the electron cloud.

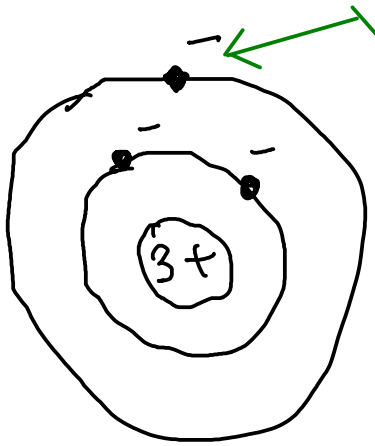
- Relates to the size of the atom.

- As you go DOWN A GROUP (↓), the atomic radius INCREASES.

  - Why? As you go down a period, you are ADDING SHELLS!

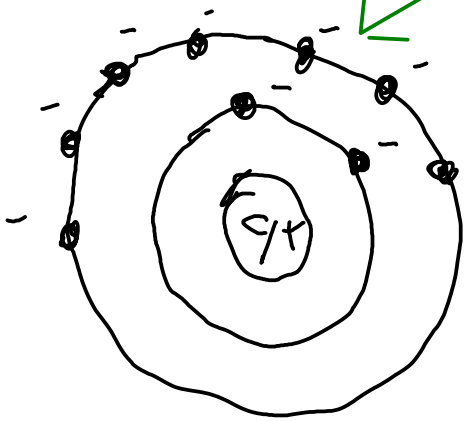
- As you go ACROSS A PERIOD (→), the atomic radius DECREASES

Why? Let's look at some sample atoms.



Outer electron sees an effective +1 charge (shielded from +3 nucleus by 2 electrons)

lithium $1s^2 2s^1$



Outer electrons see an effective +7 charge (shielded from +9 nucleus by 2 electrons)

fluorine $1s^2 2s^2 2p^5$

... so fluorine's outer shell is pulled closer to the nucleus than lithium's!

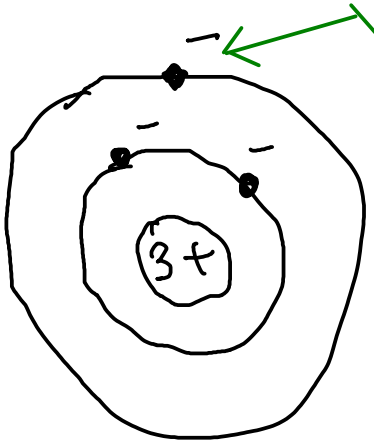
(FIRST) IONIZATION ENERGY

- The amount of energy required to remove a single electron from the outer shell of an atom.
- Relates to reactivity for metals. The easier it is to remove an electron, the more reactive the metal.
- As you go DOWN A GROUP (↓), the ionization energy DECREASES.

  - Why? As you go down a period, you are ADDING SHELLS. Since the outer electrons are farther from the nucleus and charge attraction lessens with distance, this makes electrons easier to remove as the atoms get bigger!

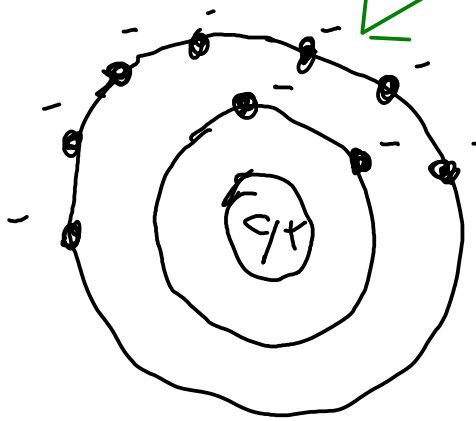
- As you go ACROSS A PERIOD (→), the ionization energy INCREASES.

  - Why? Let's look at some sample atoms.



Outer electron sees an effective +1 charge (shielded from +3 nucleus by 2 electrons)

lithium

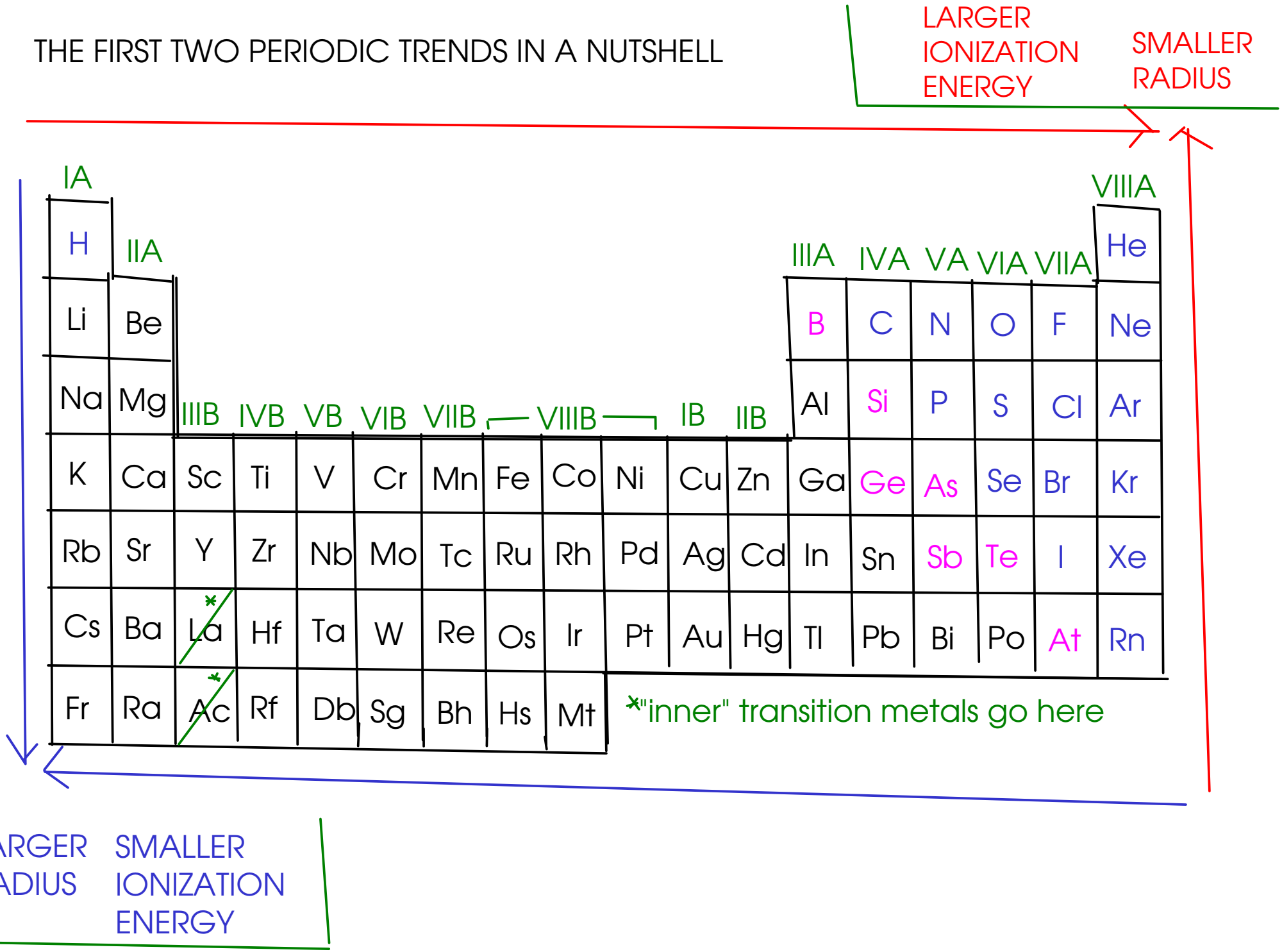


Outer electrons see an effective +7 charge (shielded from +9 nucleus by 2 electrons)

fluorine

... since fluorine's outer electrons are held on by a larger effective charge, they are more difficult to remove than lithium's.

THE FIRST TWO PERIODIC TRENDS IN A NUTSHELL



ELECTRON AFFINITY

- the electron affinity is the ENERGY CHANGE on adding a single electron to an atom.
  - Atoms with a positive electron affinity cannot form anions.
  - The more negative the electron affinity, the more stable the anion formed!

- General trend: As you move to the right on the periodic table, the electron affinity becomes more negative.

EXCEPTIONS

- Group IIA does not form anions (positive electron affinity)!

ns^2 ← valence electrons for Group IIA!

↳ period number

- To add an electron, the atom must put it into a higher-energy (p) subshell.

- Group VA: can form anions, but has a more POSITIVE electron affinity than IVA

$ns^2 np^3$ ← valence electrons for Group VA!

↳ Half-full "p" subshell! To add an electron, must start pairing!

- Group VIIIA (noble gases) does not form anions

$ns^2 np^6$

↳ full "s" and "p" subshells!

CHEMICAL BONDS

- A CHEMICAL BOND is a strong attractive force between the atoms in a compound.

3 TYPES OF CHEMICAL BOND

Type	Held together by...	Example
Ionic bonds	attractive forces between oppositely charged ions	sodium chloride
Covalent bonds	sharing of valence electrons between two atoms (sometimes more - "delocalized bonds")	water
Metallic bonds *	sharing of valence electrons with all atoms in the metal's structure - make the metal conduct electricity	any metal

*For CHM 110, you don't need to know anything more about metallic bonds than what's in this table. If you take physics, you may learn more about the characteristics of the metallic bond.

... so how can you tell what kind of bond you have? You can use the traditional rules of thumb:

- Metal-Nonmetal bonds will be ionic
- Nonmetal-nonmetal bonds are usually covalent

Metalloids act like NONMETALS, here.

... but for better information about bonding, you can use ELECTRONEGATIVITY.

ELECTRONEGATIVITY:
-A measure of how closely to itself an atom will hold shared electrons

p346: chart of electroneg. values

p352, 10th

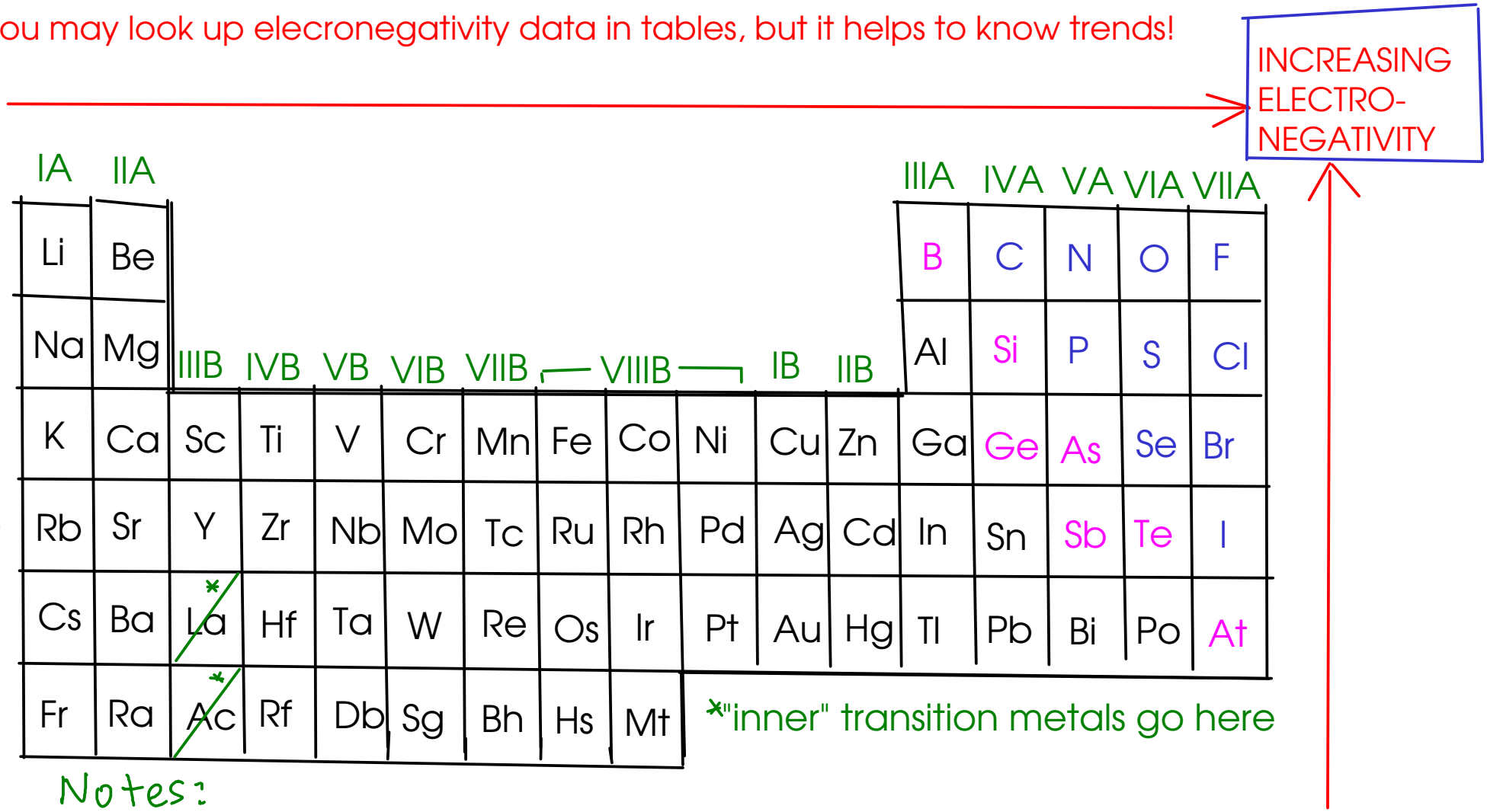
... in other words, how ELECTRON-GREEDY an atom is!

Bonds with ...	are ...	Examples
Little or no difference in electronegativity between atoms	NONPOLAR COVALENT	C-C, C-H, etc.
Larger differences in electronegativity between atoms	* POLAR COVALENT	H-F, C-F, C-Cl, etc.
Very large differences in electronegativity between atoms	IONIC	NaCl, KBr, etc.

* A POLAR bond is a bond where electrons are shared unevenly - electrons spend more time around one atom than another, resulting in a bond with slightly charged ends

ELECTRONEGATIVITY TRENDS

- You may look up elecronegativity data in tables, but it helps to know trends!



Notes:

① - FLUORINE is the most elecronegative element, while FRANCIUM is the least!

② - All the METALS have low electronegativity

③ - HYDROGEN is similar in electronegativity to CARBON

... so C-H bonds are NONPOLAR

(p 346)

DESCRIBING CHEMICAL BONDING

"octet rule"

- a "rule of thumb" (NOT a scienfitic law) predicting how atoms will exchange or share electrons to form chemical compounds

- atoms will gain, lose, or share enough electrons so that they end up with full "s" and "p" subshells in their outermost shell.

- Why "octet"? An "s" subshell can hold two electrons, while a "p" subshell can hold six. 2+6 = 8

IONIC COMPOUNDS

- When atoms react to form IONS, they GAIN or LOSE enough electrons to end up with full "s" and "p" subshells.

example:

$Al + 3\,Br \rightarrow$

$[Ne]3s^2 3p^1$ → $[Ar]3d^{10}4s^2 4p^5$

$[Ar]3d^{10}4s^2 4p^5$

$[Ar]3d^{10}4s^2 4p^5$

Aluminum loses its outer three electrons, and each bromine gains one!

$AlBr_3$ ↙ $1s^2 2s^2 2p^6$

Al^{3+} : $[Ne]$

Br^- : $[Ar]3d^{10}4s^2 4p^6$

Br^- : $[Ar]3d^{10}4s^2 4p^6$

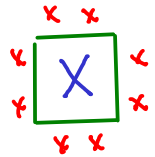
Br^- : $[Ar]3d^{10}4s^2 4p^6$

... but using electron configurations to describe how aluminum bromide forms is a bit cumbersome! Can we simplify the picture a bit?

LEWIS NOTATION / ELECTRON-DOT NOTATION

- Lewis notation represents each VALENCE electron with a DOT drawn around the atomic symbol. Since the valence shell of an atom contains only "s" and "p" electrons, the maximum number of dots drawn will be EIGHT.

- To use electron-dot notation, put a dot for each valence electron around the atomic symbol. Put one dot on each "side" of the symbol (4 sides), then pair the dots for atoms that have more than four valence electrons.



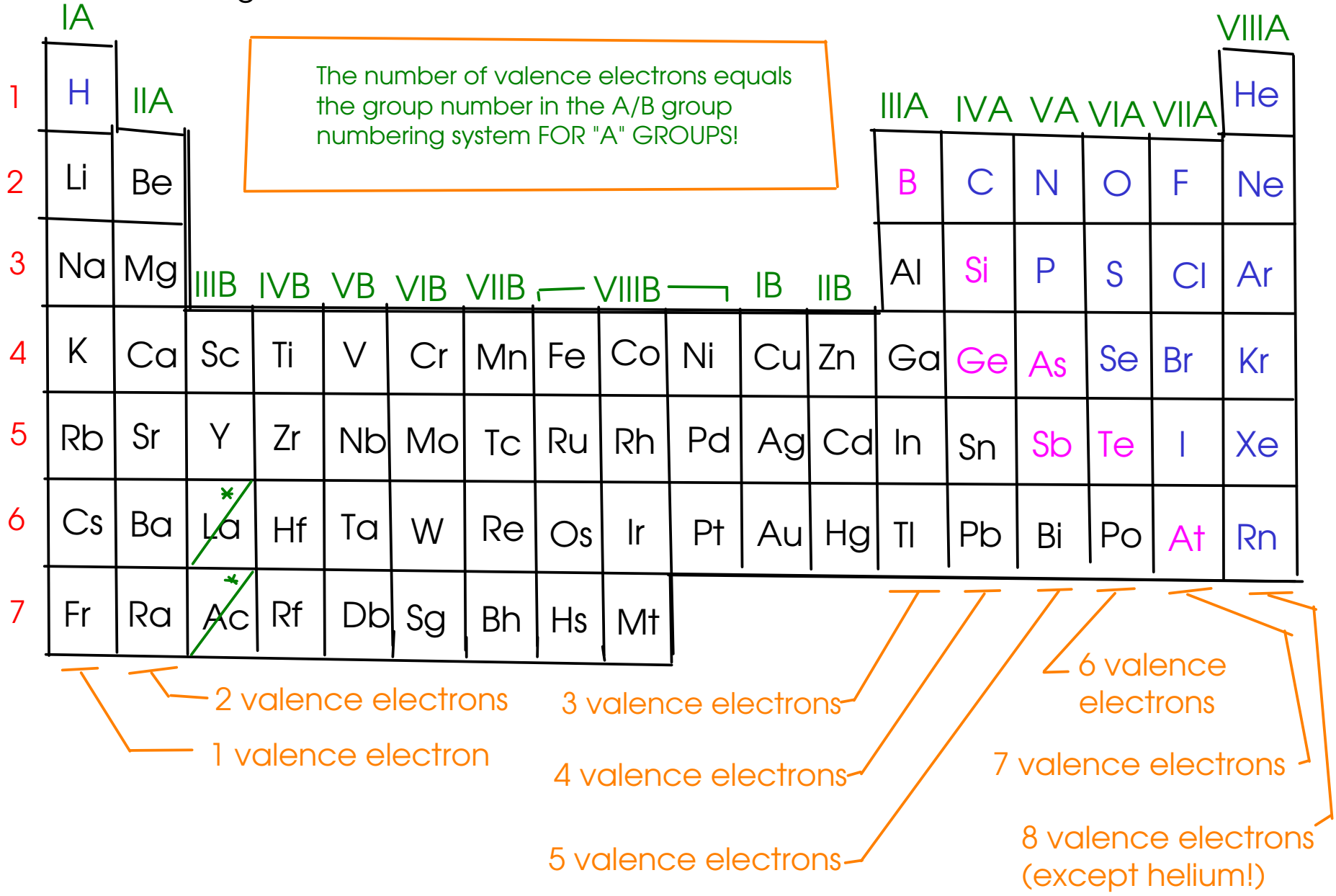
examples:

More examples

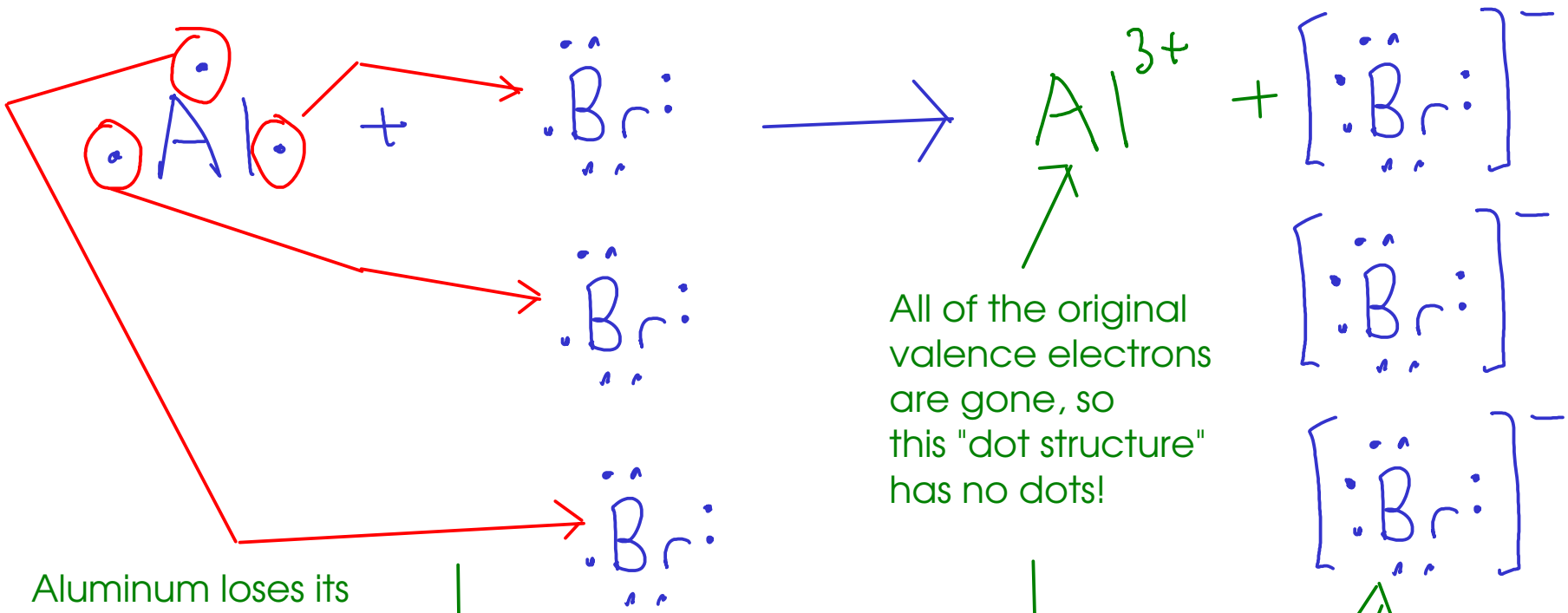
Which "side" you draw the dots on isn't important, as long as you have the right number of electrons and the right number of "pairs"

.. . are all equivalent!

To draw a dot structure for an atom, you need to know HOW MANY valence electrons it has! You can determine this simply from the periodic table, WITHOUT writing the whole electron configuration!



... but how do we use this to describe a reaction that produces ions? Let's look at our previous example!



All of the original valence electrons are gone, so this "dot structure" has no dots!

Each bromide ion has eight outer electrons!

Aluminum loses its outer three electrons (in the 3s and 3p subshells) (leaving it with full 2s and 2p subshells.

Aluminum is oxidized!

Each bromine atom requires one more electron to get a total of eight outer electrons (full "s" and "p" subshells)

Bromine is reduced!

Redox reactions are much clearer when seen using dot notation!

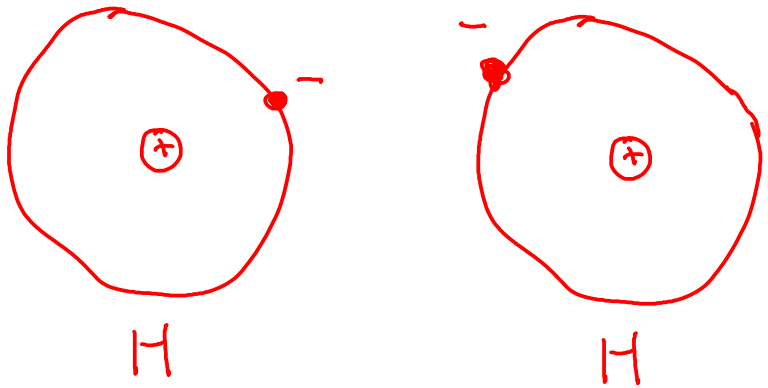
... this is a bit easier to follow than looking at all those letters and numbers in the electron configurations for these elements!

MOLECULAR COMPOUNDS

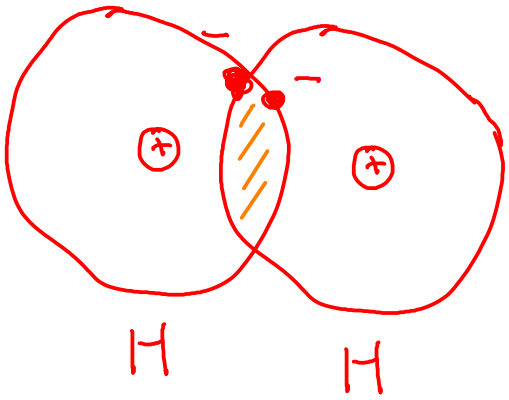
- Form when atoms SHARE electrons instead of transferring them. This results in the formation of MOLECULES ... groups of atoms held together by electron-sharing.

How might atoms SHARE electrons? By coming together close enough so that their atomic ORBITALS overlap each other:

This idea is called VALENCE BOND THEORY!



Each hydrogen atom has a single electron in a 1s orbital.

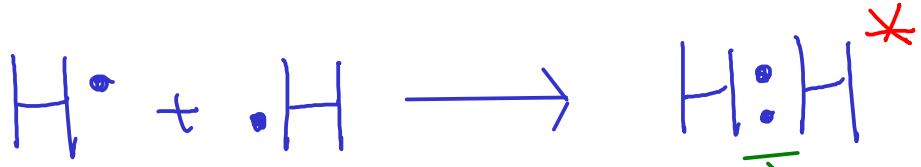


When hydrogen atoms come close enough to each other for these orbitals to OVERLAP, each hydrogen "sees" BOTH electrons, filling up the "s" orbitals of both atoms. This is a COVALENT BOND.

Co: together
Valent: valence shells

This is the DIATOMIC MOLECULE, H_2

... so how would this look using dot notation?

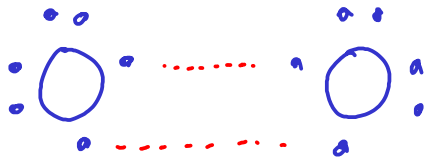


a single shared pair of electrons.
This is called a SINGLE BOND

In dot structures, SHARED PAIRS of electrons are often written as DASHES to make the structures look neater.

* Why doesn't hydrogen end up with eight electrons? Because hydrogen has only the first shell, which contains only a single "s" subshell (NO "p" subshell). This "s" subshell is full with two electrons, and that's all hydrogen needs to get.

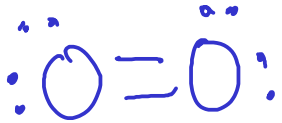
Let's look at OXYGEN ...



We know that oxygen exists in air as the diatomic molecule O_2

The oxygen atoms share TWO pairs of electrons. This is called a DOUBLE BOND

OR



Each oxygen atom has a share in eight electrons!

A few notes on the double bond:

1. - For atoms to share more than one pair of electrons, they have to move closer to one another than they would if they were only sharing one pair of electrons. This BOND DISTANCE is measurable!

2. - It takes more energy to break a double bond between two atoms than it would to break a single bond between the same two atoms. This BOND ENERGY is also measurable!