

Quantum mechanics treats the electrons as waves and models THAT behavior!

- To describe the electrons, we use WAVEFUNCTIONs - which are mathematical descriptions of the behavior of electrons.
- The wavefunction describes the probability of finding an electron in a given space
- For larger objects, the wave behavior isn't very important and quantum mechanics becomes traditional Newtonian physics.

When we talk about describing electrons ... we will talk about the PARAMETERS that go into this WAVEFUNCTION ... without doing the actual math.

- There are FOUR of these parameters. (the Bohr model had only one!)
- The parameters are called "quantum numbers"
 - ① Principal quantum number
 - ② Angular momentum quantum number
 - ③ Magnetic quantum number
 - ④ Spin quantum number

- 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.

$$n = 1, 2, 3, 4, \dots \text{ (integers)}$$

② ANGULAR MOMENTUM QUANTUM NUMBER: l

- "subshell"

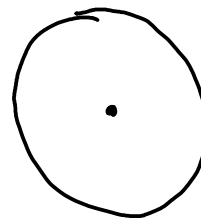
- Represents the SHAPE of the region of space where the electron is found.

- (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

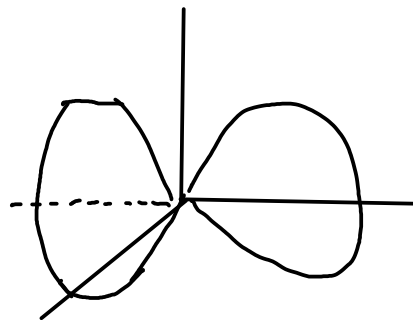
$n=1$; $l=0$



"l" = 0 ; spherical subshell

Also called an "s" subshell.

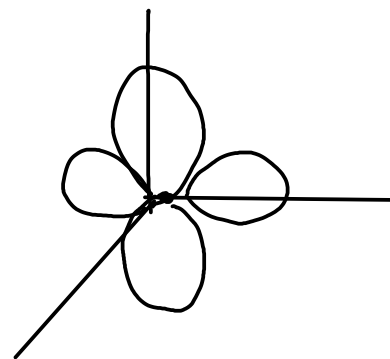
$n=2$; $l=0, 1$



"l" = 1 ; dumbbell shaped

Also called a "p" subshell

$n=3$, $l=0, 1, 2$



"l" = 2 ; flower-shaped

Also called a "d" subshell

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. (p285, 3-D pictures of subshells)

$l=0$ "s"

$l=2$ "d"

$l=4$ "g"

$l=1$ "p"

$l=3$ "f"

↓ The rest follow the alphabet

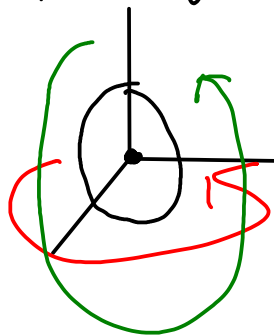
③ MAGNETIC QUANTUM NUMBER m_l

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

$$m_l = -l \text{ to } +l, \text{ integers}$$

$$l = 0, m_l = 0$$

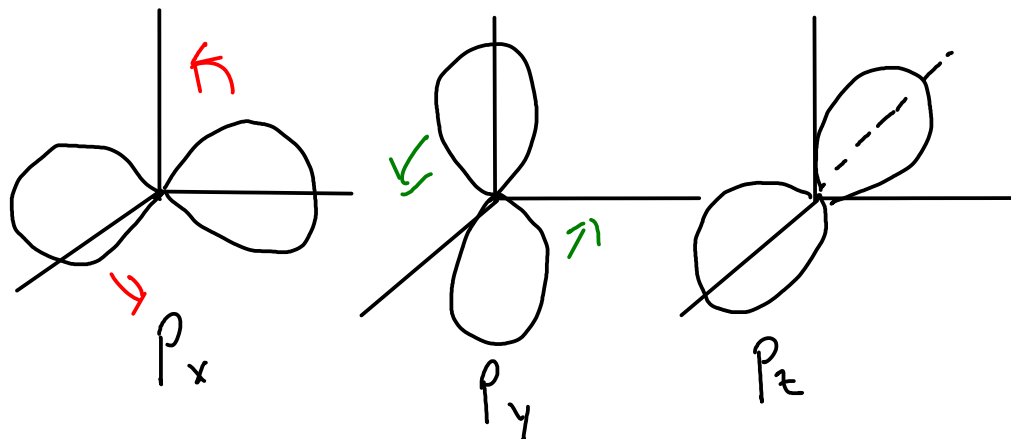
"s"



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

$$l = 1, m_l = -1, 0, 1$$

"p"



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

$$l = 2, m_l = -2, -1, 0, 1, 2 \text{ (five orientations)}$$

"d"

picture
p285,
p290 (tent)

$$l = 3, m_l = -3, -2, -1, 0, 1, 2, 3 \text{ (seven orientations)}$$

"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.

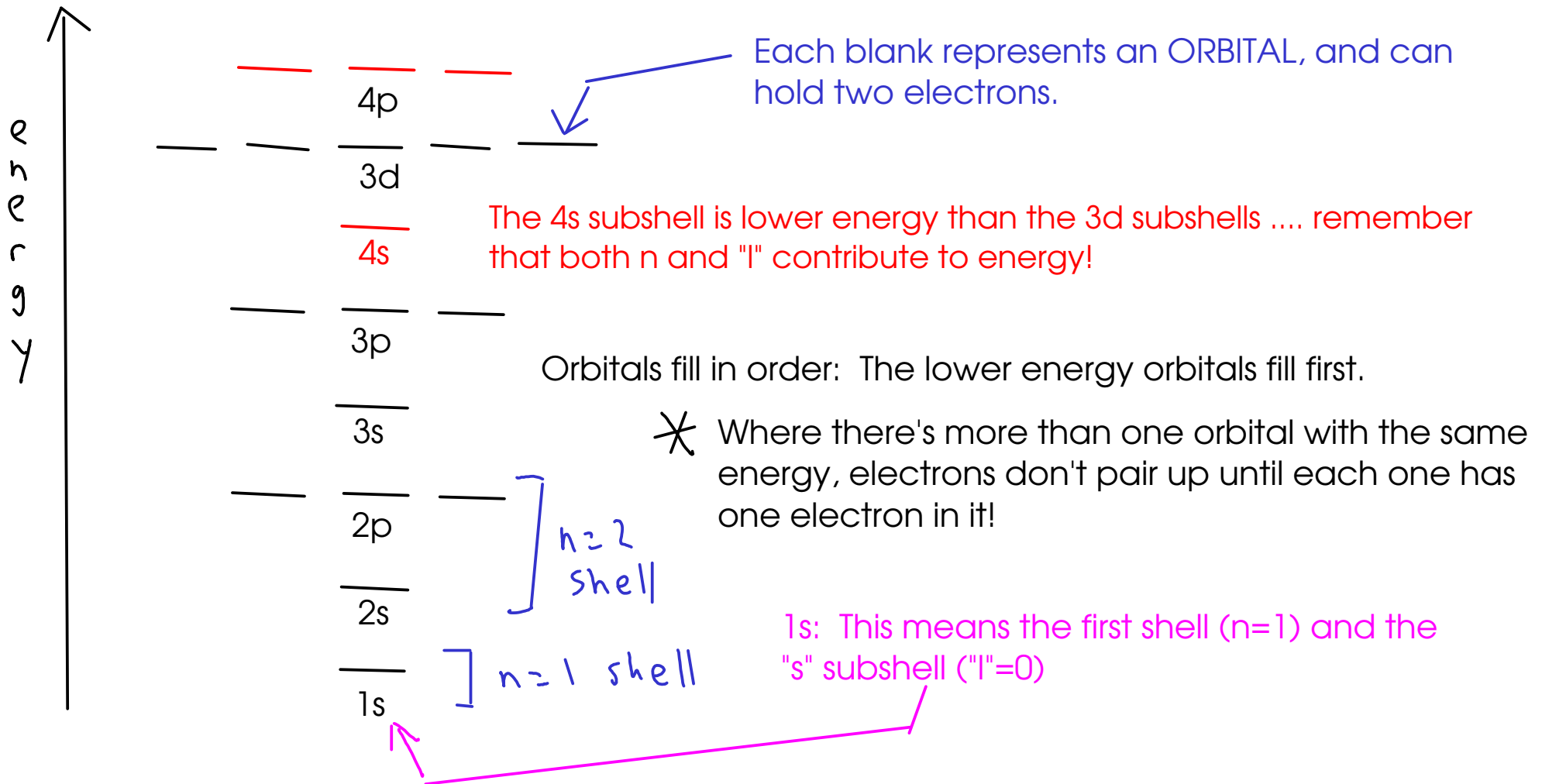
④ (MAGNETIC) SPIN QUANTUM NUMBER: m_s

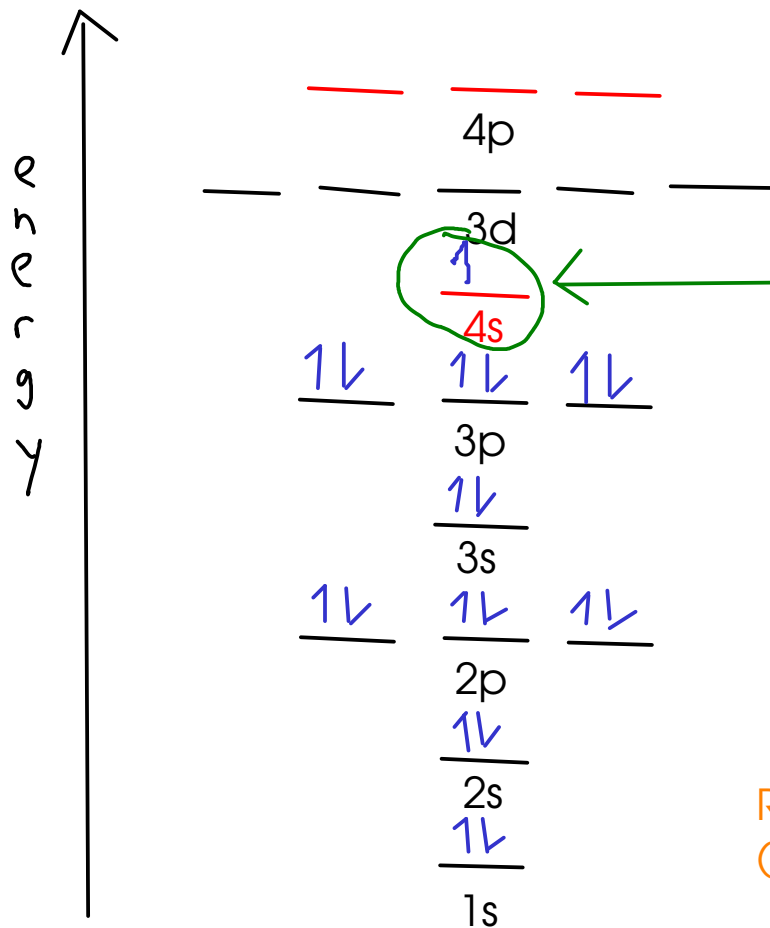
$$m_s = -\frac{1}{2} \text{ OR } +\frac{1}{2} \quad \text{"spin down" or "spin up"}$$

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

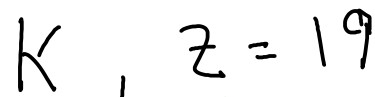
ORBITAL DIAGRAM

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





How would an orbital diagram for the element POTASSIUM look?



atomic number

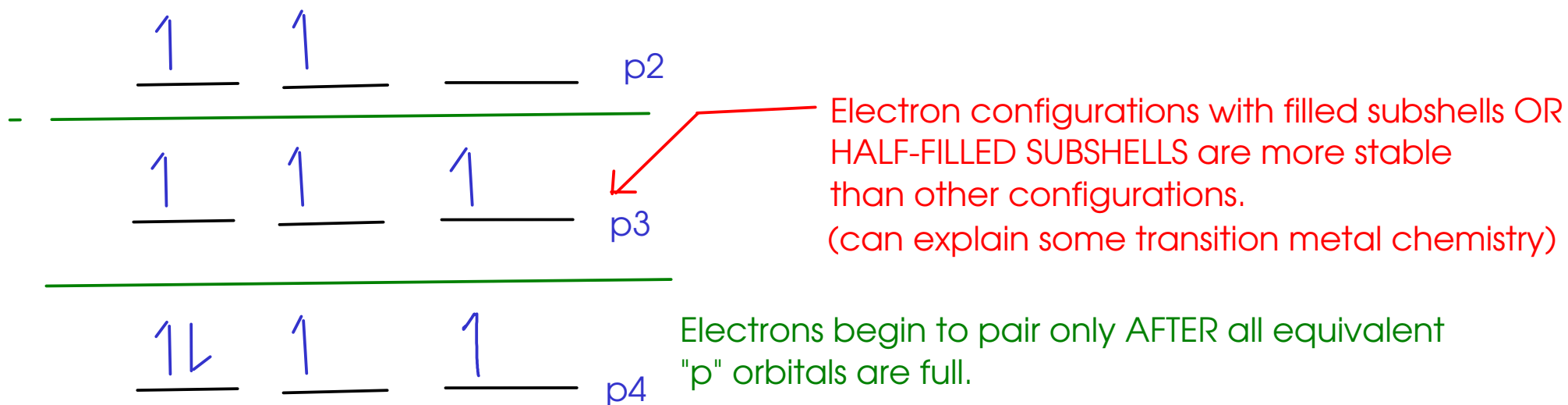
Electrons in the outermost shell of an atom are called VALENCE electrons. THESE electrons are normally involved in chemical bonding.

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.

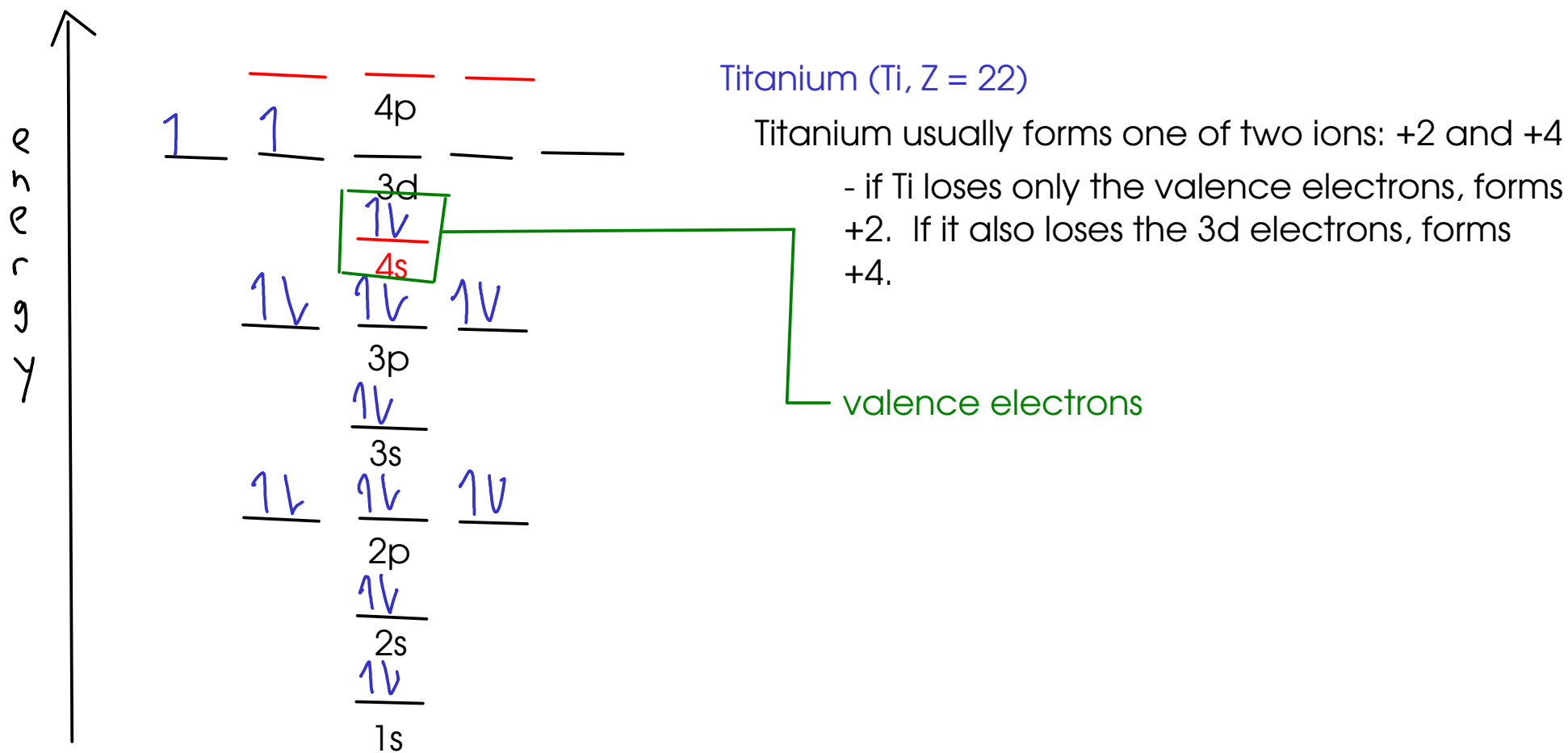


Experimental evidence for Hund's rule:

"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.

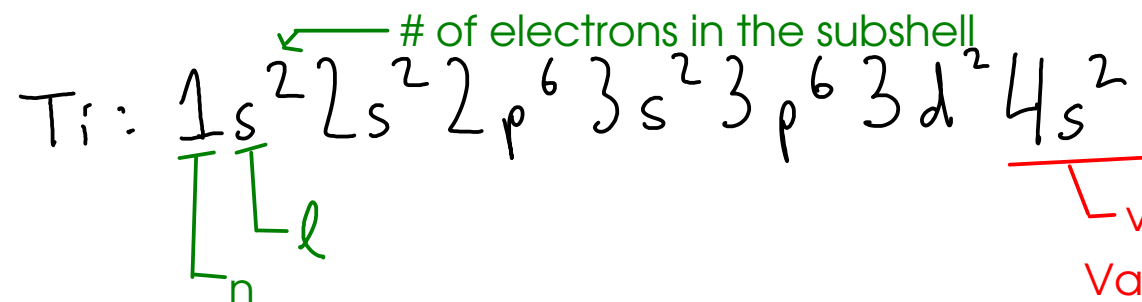
A little bit about transition metals...



- 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".



valence electrons

Valence electrons have the largest value for "n"!



valence electrons

"noble gas core". We're saying that titanium has the same electron configuration as argon does, with the addition of the electrons that follow. This is a useful shorthand, since the "core" electrons generally don't get involved in bonding.

ELECTRON CONFIGURATION AND THE PERIODIC TABLE

IA												VIII A													
IA	IIA											III A	IV A	V A	VI A	VII A	VIII A								
H	He																								
Li	Be											B	C	N	O	F	Ne								
Na	Mg	III B	IV B	V B	V I B	V II B	V III B	I B	I I B											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr								
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe								
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn								
Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt	*"inner" transition metals go here																

"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!

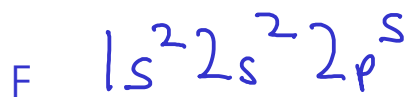
1	IA H											VIIIA He						
2	Li	IIA Be											IIIA B	IVA C	V N	VIA O	VIIA F	VIIIA Ne
3	Na	Mg	IIIB	IVB	VB	VIB	VIIB	VIIIB	IB	IIB	Al	Si	P	S	Cl	Ar		
4	K _{4s}	Ca	Sc _{3d}	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga _{4p}	Ge	As	Se	Br	Kr
5	Rb	Sr	Y _{4d}	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La _{5d}	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac _{6d}	Rf	Db	Sg	Bh	Hs	Mt	*"inner" transition metals go here								

"d" block: The d block is shifted DOWN.!

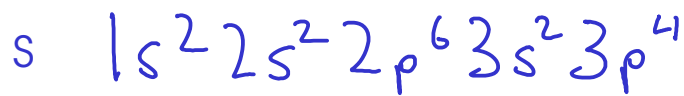
Example: Phosphorus (P): $1s^2 2s^2 2p^6 3s^2 3p^3$

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

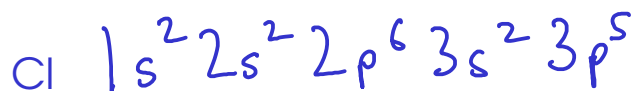
EXAMPLES:



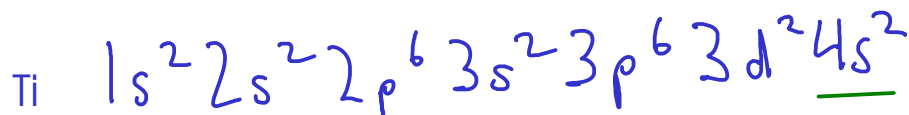
Remember - valence electrons are ALL of the electrons in the outermost SHELL (n)! More that one subshell (l) may be included in the valence electrons



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!



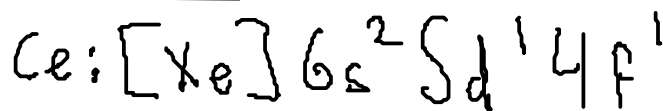
You can order the subshells in numeric order OR in filling order



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



Sample f-block element



PERIODIC TRENDS

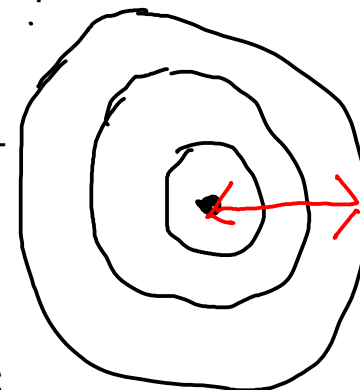
- Some properties of elements can be related to their positions on the periodic table.

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.

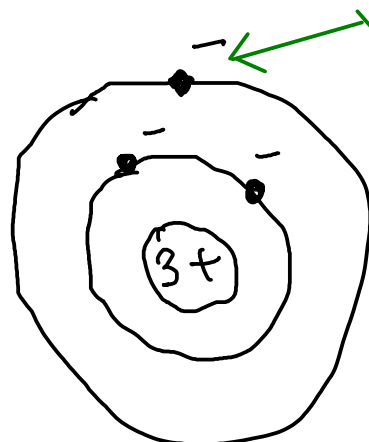
- As you go DOWN A GROUP (↓), the atomic radius INCREASES.



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

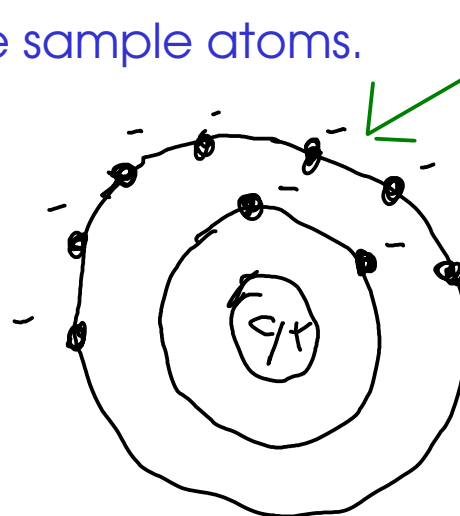
- As you go ACROSS A PERIOD (→), the atomic radius DECREASES

Why? Let's look at some sample atoms.



lithium $1s^2 2s^1$

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



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

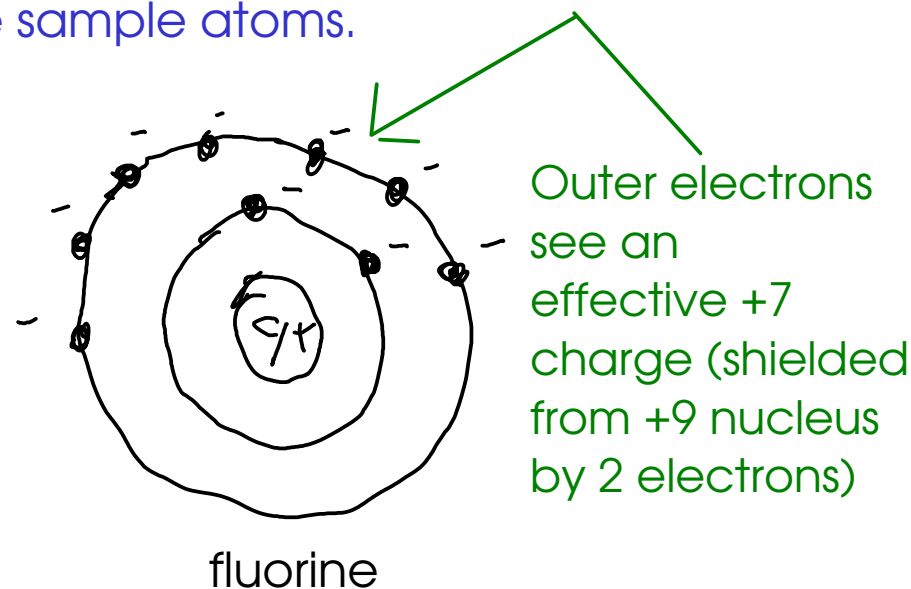
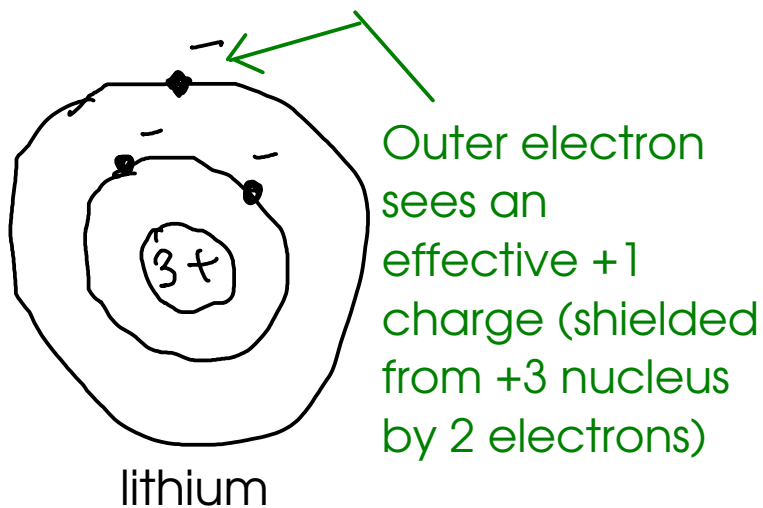
Outer electrons see an effective +7 charge (shielded from +9 nucleus by 2 electrons)

... 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.



... 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

LARGER
IONIZATION
ENERGYSMALLER
RADIUS

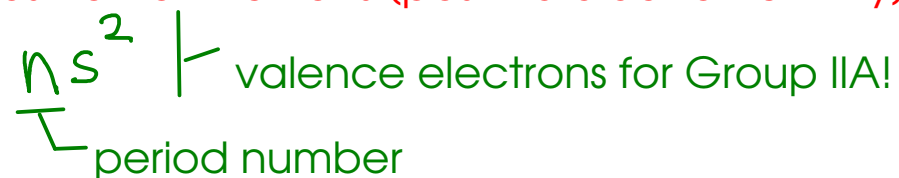
IA																			VIIIA
H																			He
	IIA											IIIA	IVA	VA	VIA	VIIA			
Li	Be											B	C	N	O	F			Ne
Na	Mg	IIIB	IVB	VB	VIB	VII B	VIII B	IB	IIB			Al	Si	P	S	Cl			Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br			Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I			Xe
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At			Rn
Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt	*"inner" transition metals go here										

LARGER
RADIUS
SMALLER
IONIZATION
ENERGY

- 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.

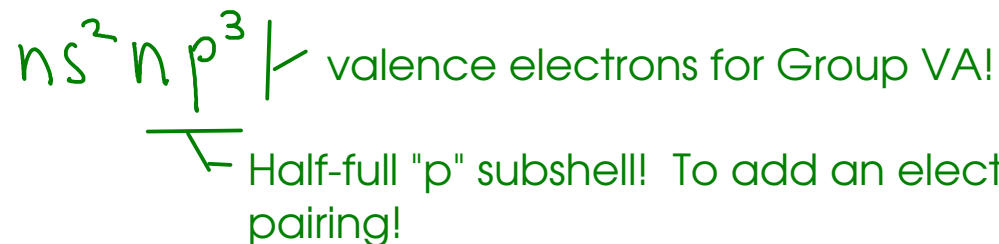
EXCEPTIONS

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



- 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



- Group VIIIA (noble gases) does not form anions



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
<u>Covalent</u> 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

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

	IA	IIA										IIIA	IVA	VA	VIA	VIIA	
2	Li	Be										B	C	N	O	F	
3	Na	Mg	IIIB	IVB	VB	VIB	VIIB	VIIIB	IB	IIB		Al	Si	P	S	Cl	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt	*"inner" transition metals go here							

Notes:

- ① - FLUORINE is the most electronegative element, while FRANCIUM is the least!
- ② - All the METALS have low electronegativity
- ③ - HYDROGEN is similar in electronegativity to CARBON

(p 346)

... so C-H bonds are NONPOLAR