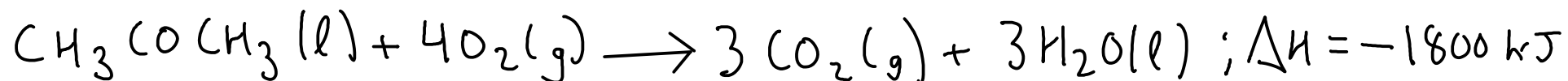


<sup>157</sup> SINCE the enthalpy change does NOT depend on path, this means that we can use standard values for enthalpy to predict the heat change in reactions that we have not tested in a calorimeter.

---

## THERMOCHEMICAL EQUATIONS

- is like a regular chemical equation, except that phase labels are REQUIRED and the enthalpy for the reaction is given along with the equation.



- Why are phase labels required? Because phase changes either absorb or release energy.

$\Delta H = -1800 \text{ kJ}$  ... what does this mean?

$$1 \text{ mol CH}_3\text{COCH}_3 = -1800 \text{ kJ}$$

$$4 \text{ mol O}_2 = -1800 \text{ kJ}$$

$$3 \text{ mol CO}_2 = -1800 \text{ kJ}$$

$$3 \text{ mol H}_2\text{O} = -1800 \text{ kJ}$$

We treat the enthalpy change as if it's another product of the reaction!



What would be the enthalpy change when 25 g of water are produced by the reaction?

1 - Convert 25 grams of water to moles. Use FORMULA WEIGHT.

2 - Convert moles water to enthalpy change. Use THERMOCHEMICAL EQUATION.

$$\textcircled{1} \text{H}_2\text{O} - \text{H}: 2 \times 1.008$$

$$\text{O}: 1 \times 16.00$$

$$\underline{18.016 \text{ g H}_2\text{O} = \text{mol H}_2\text{O}}$$

$$\textcircled{2} 3 \text{ mol H}_2\text{O} = -1800 \text{ kJ}$$

$$25 \text{ g H}_2\text{O} \times \frac{\textcircled{1} \text{ mol H}_2\text{O}}{18.016 \text{ g H}_2\text{O}} \times \frac{\textcircled{2} -1800 \text{ kJ}}{3 \text{ mol H}_2\text{O}} = \boxed{-830 \text{ kJ}}$$

\* This is an EXOTHERMIC process (negative enthalpy change). Energy is LEAVING the system.

\* As long as we're at constant pressure, -830 kJ also equals Q, the heat.

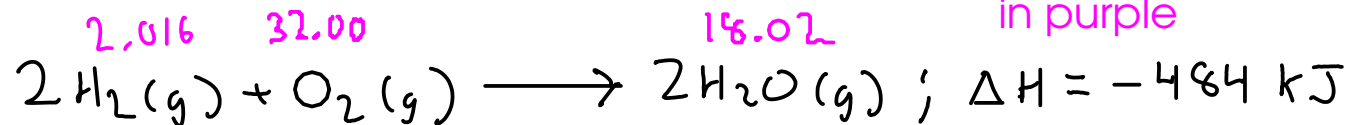
A few more terms related to enthalpy:

- Enthalpy of vaporization / heat of vaporization: The enthalpy change on vaporizing one mole of a substance. (from liquid to vapor)

- Enthalpy of fusion / heat of fusion: The enthalpy change when a mole of liquid changes to the solid state.



Phase changes require energy, too!



Calculate the enthalpy change for the combustion of 1000. g of hydrogen gas.

1 - Convert 1000. g hydrogen gas to moles. Use FORMULA WEIGHT.

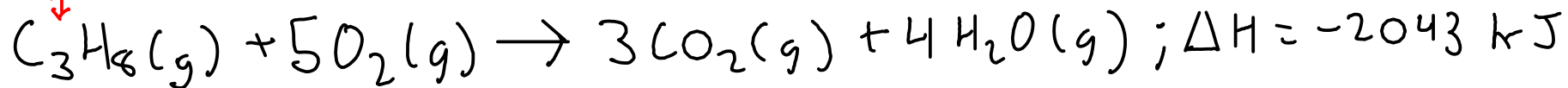
2 - Convert moles hydrogen gas to enthalpy change. Use THERMOCHEMICAL EQUATION.

$$\textcircled{1} 2.016 \text{ g H}_2 = \text{mol H}_2 \quad \textcircled{2} 2 \text{ mol H}_2 = -484 \text{ kJ}$$

$$1000. \text{ g H}_2 \times \frac{\text{mol H}_2}{2.016 \text{ g H}_2} \times \frac{-484 \text{ kJ}}{2 \text{ mol H}_2} = \boxed{-120000 \text{ kJ}} \text{ per } 1000. \text{ g H}_2$$

$\textcircled{1}$ 
 $\textcircled{2}$

propane



Calculate the volume of propane gas at 25.0 C and 1.08 atm required to provide 565 kJ of heat using the reaction above.

1 - Convert 565 kJ of heat to moles propane gas. Use THERMOCHEMICAL EQUATION.

2 - Convert moles propane to volume. Use IDEAL GAS EQUATION,  $PV=nRT$

$$\textcircled{1} \text{ mol } \text{C}_3\text{H}_8 = -2043 \text{ kJ}$$

$$-565 \text{ kJ} \times \frac{\text{mol } \text{C}_3\text{H}_8}{-2043 \text{ kJ}} = 0.2765540871 \text{ mol } \text{C}_3\text{H}_8$$

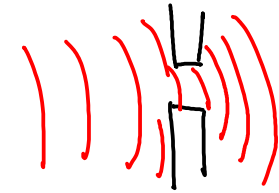
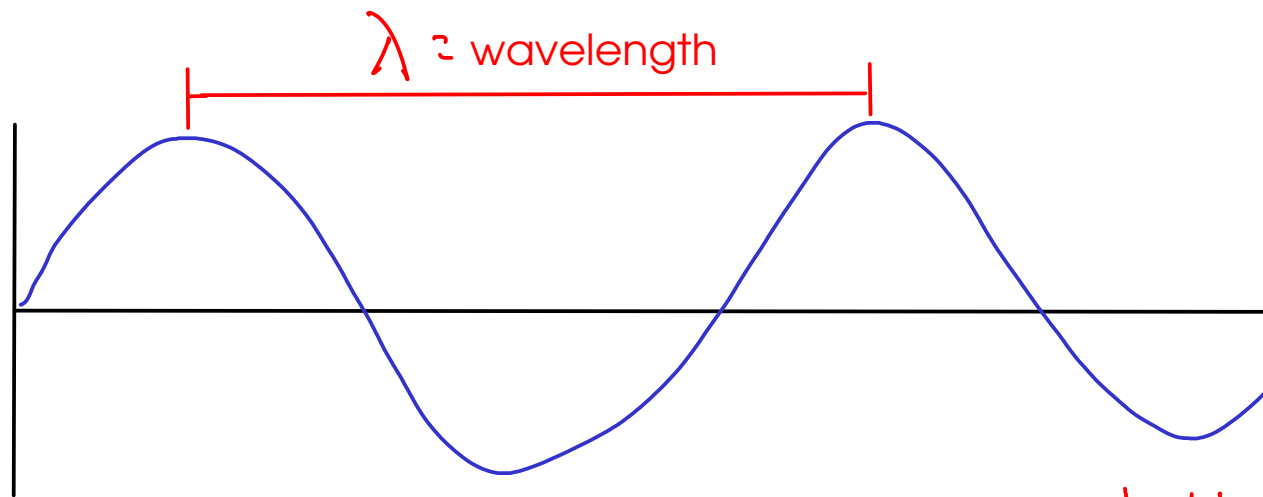
\* This heat is NEGATIVE because the reaction is providing (in other words ... losing) this amount of heat, and we're calculating based on the reaction.

$$\textcircled{2} \begin{array}{l} PV=nRT \\ V = \frac{nRT}{P} \end{array} \quad \left| \quad \begin{array}{l} n = 0.2765540871 \text{ mol } \text{C}_3\text{H}_8 \\ T = 25.0^\circ\text{C} = 298.2 \text{ K} \\ P = 1.08 \text{ atm} \end{array} \quad R = 0.08206 \frac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}$$

$$V = \frac{(0.2765540871 \text{ mol } \text{C}_3\text{H}_8)(0.08206 \frac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}})(298.2 \text{ K})}{1.08 \text{ atm}} = 6.27 \text{ L } \text{C}_3\text{H}_8 \text{ at } 25.0^\circ\text{C}, 1.08 \text{ atm}$$

## END OF CHAPTER 6

## LIGHT



Diffraction

frequency = wavelengths / time =  $\nu$      $s^{-1}$ : Hertz, Hz

- Light has properties of WAVES such as DIFFRACTION (it bends around small obstructions).
- Einstein noted that viewing light as a particle that carried an energy proportional to the FREQUENCY could explain the PHOTOELECTRIC EFFECT!

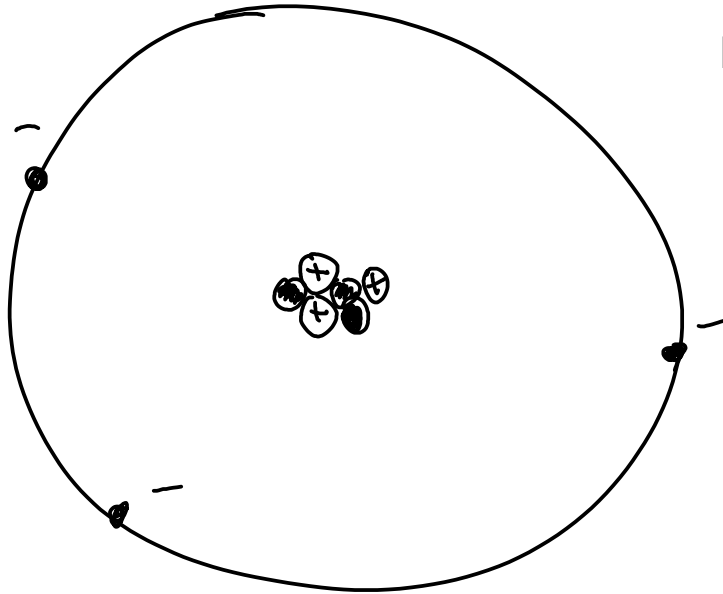
$$E_{\text{photon}} = h \nu$$

Planck's constant:  $6.63 \times 10^{-34} \text{ J}\cdot\text{s}$

photon = particle or packet of light

(The photoelectric effect is the emission of electrons from a metal caused by exposure to light. Einstein discovered that if the light were not of the correct FREQUENCY, increasing the INTENSITY of the light would not cause electron emission. He concluded that individual photons must have enough energy to excite an electron - i.e. they must have the appropriate frequency.)

The photoelectric effect and Einstein's ideas about the energy content of light led us to discover a new model for the atom! How? Let's start with the nuclear model:



Nuclear model:

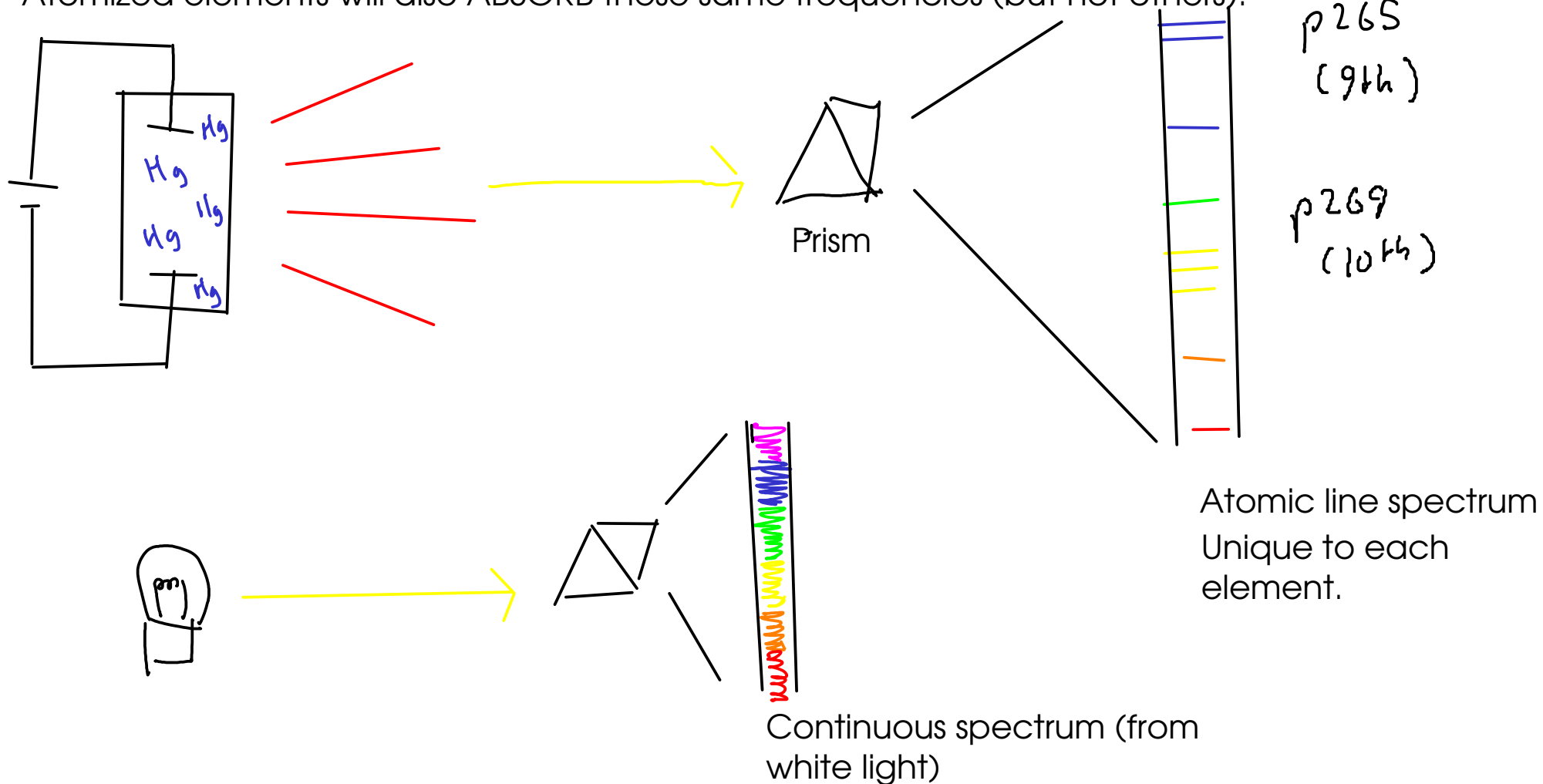
- Protons and neutrons in a dense NUCLEUS at center of atom
- Electrons in a diffuse (mostly empty) ELECTRON CLOUD surrounding NUCLEUS.

... so what's wrong with the nuclear model? Among other things, it doesn't explain ...

## ATOMIC LINE SPECTRA

- if you take element and ATOMIZE it, if excited by energy it will emit light at unique frequencies. The set of emitted frequencies is called an ATOMIC LINE SPECTRUM.

- Atomized elements will also ABSORB these same frequencies (but not others)!

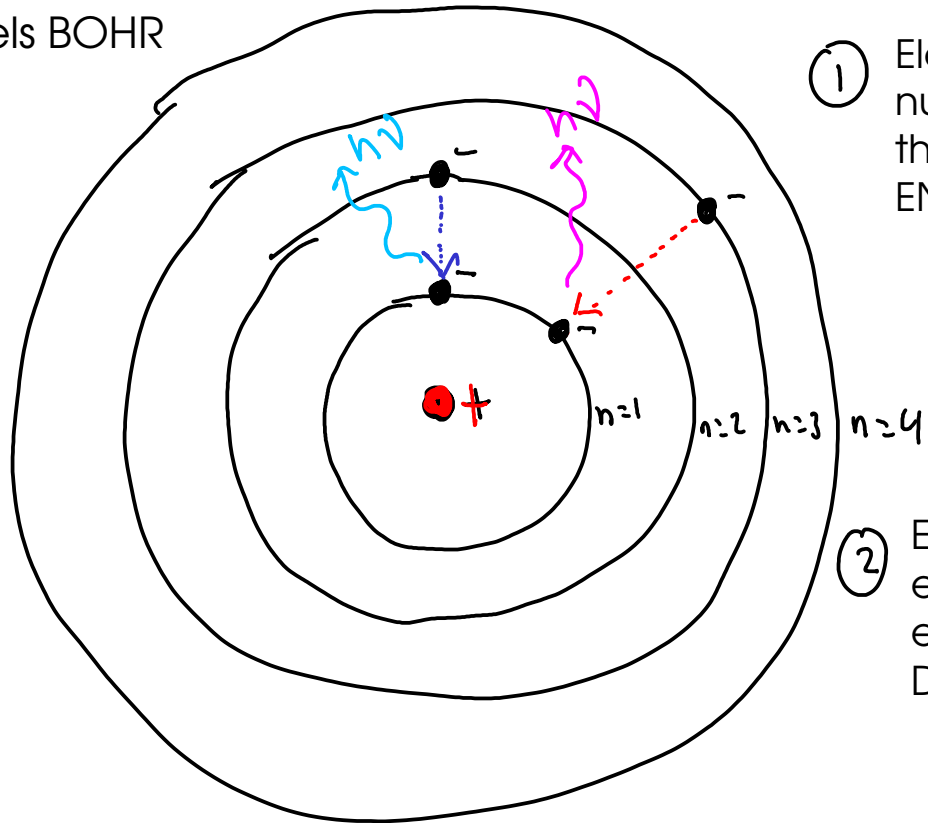


... so, why don't atoms by themselves emit continuous spectra like a flashlight would?



- The regular patterns of emission and absorption of light by atoms suggest that the electron cloud has some sort of regular structure. The specific frequencies of light emitted and absorbed relate to specific values of ENERGY in the electron cloud.

Niels BOHR

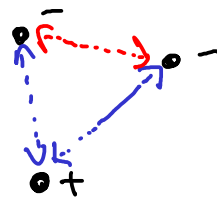


① Electrons can't be just ANYWHERE around a nucleus. They can exist only at certain distances from the nucleus. These distances correspond to certain ENERGIES and are called ENERGY LEVELS!

② Electrons CAN move (transition) between different energy levels by gaining or losing exactly enough energy to get into the new energy level. This was a DIRECT transition .

Bohr's model was the first proposal that predicted the existence of atomic line spectra, and it exactly predicted the spectra of hydrogen and "hydrogen-like" (i.e. one-electron) species.

The spectra were "off" for multi-electron atoms.



Multi-electron atoms have interactions between electrons, not just interactions between electrons and nucleus!

- The additional interactions in multi-electron atoms introduced added complexity to the model of the atom! Bohr's model was too simple.

- Improvements in Bohr's model came from treating electrons as WAVES.

de Broglie relationship

$$\lambda = \frac{h}{m \times v}$$

Planck's constant

velocity (m/s)

mass

wavelength

Calculates the WAVELENGTH of ... matter?

... for very large particles, the wavelength is very small.

- 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"

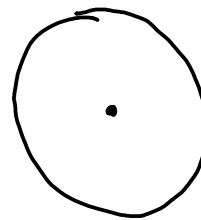
- Represents the SHAPE of the region of space where the electron is found.

- (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

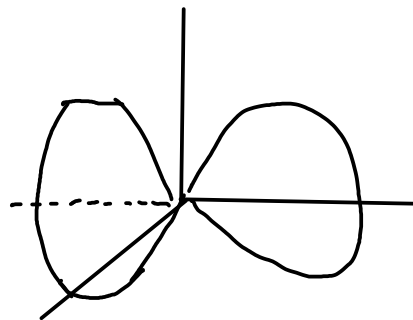
$n=1$ ;  $l=0$



" $l$ " = 0 ; spherical subshell

Also called an "s" subshell.

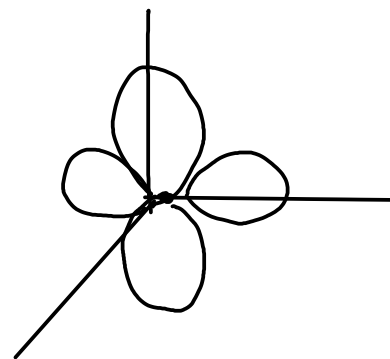
$n=2$ ;  $l=0, 1$



" $l$ " = 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. (p288, 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

(p290, 10th ed)

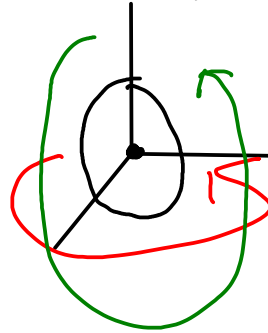
### ③ MAGNETIC QUANTUM NUMBER $m_l$

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

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

$$l = 0, m_l = 0$$

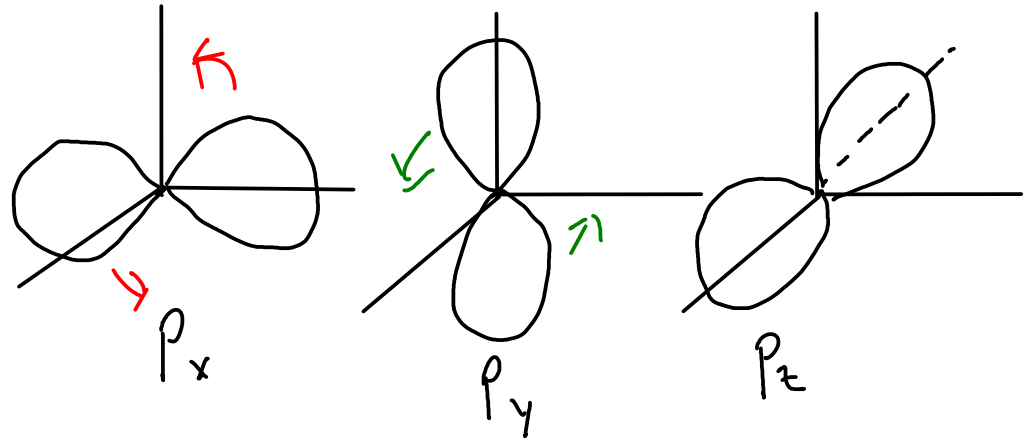
"s"



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.

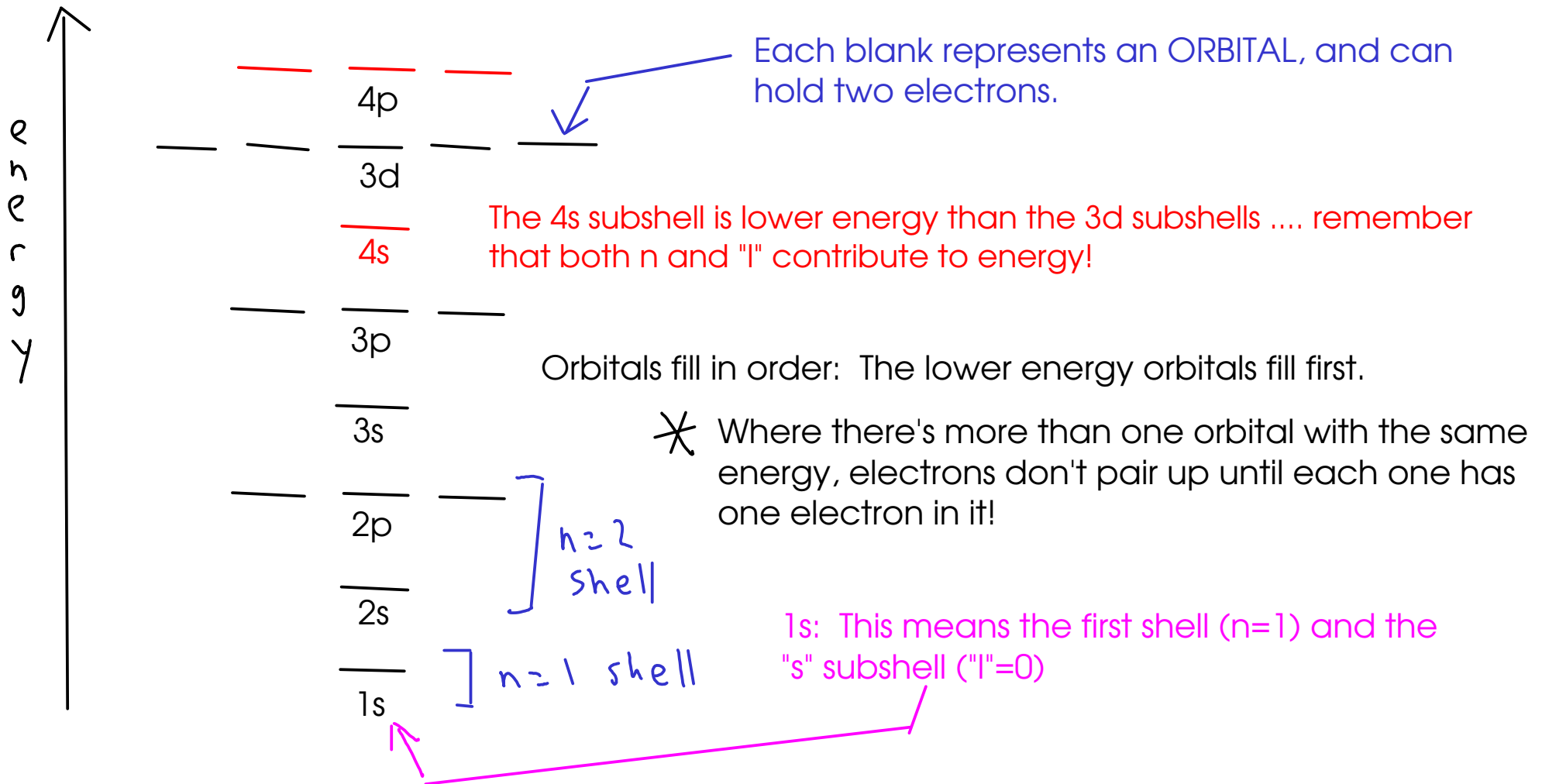
④ (MAGNETIC) SPIN QUANTUM NUMBER:  $m_s$

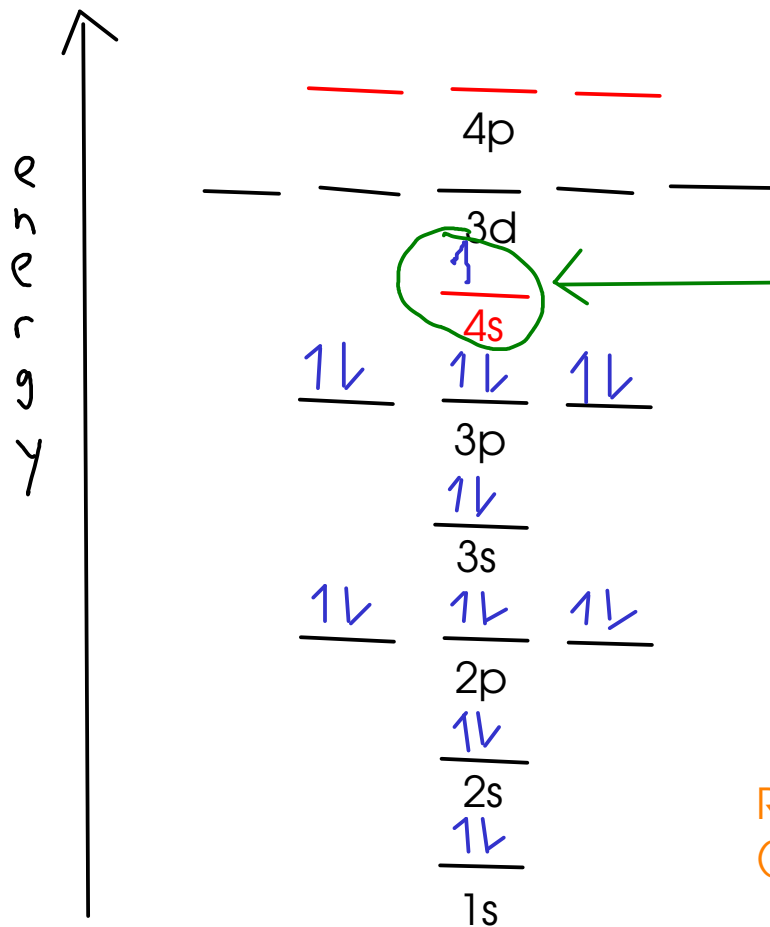
$$m_s = -\frac{1}{2} \text{ OR } +\frac{1}{2} \quad \text{"spin down" or "spin up"}$$

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

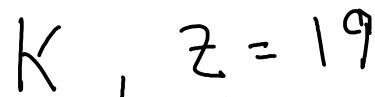
## ORBITAL DIAGRAM

- 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.

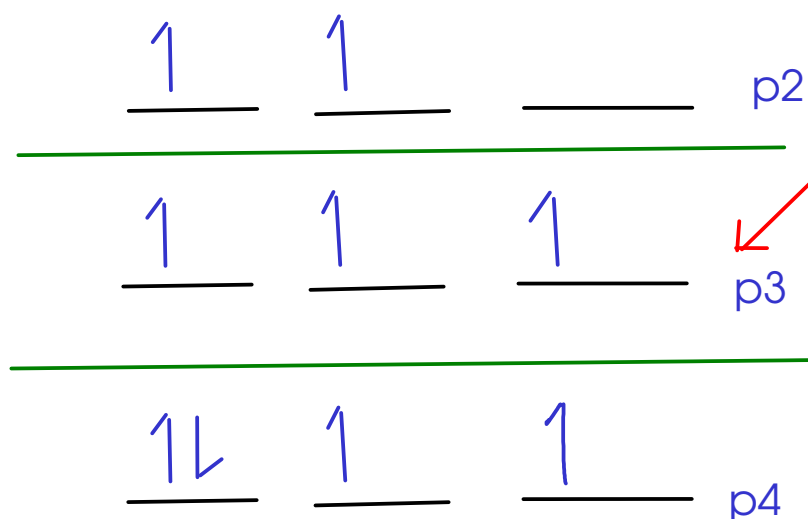
Remember: Potassium tends to lose a single electron (forming a cation) in chemical reactions.  $K^+$

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.



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

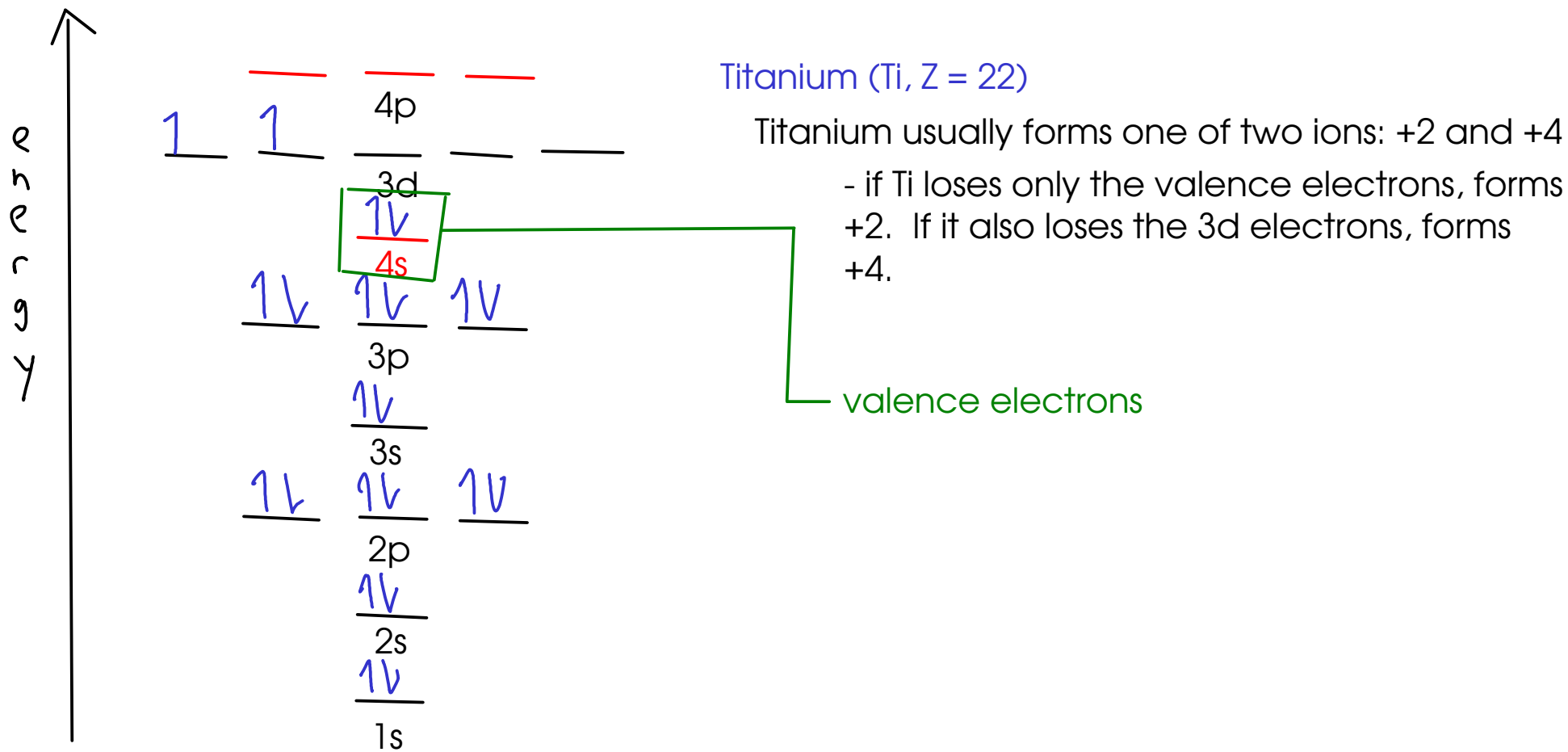
Electrons begin to pair only AFTER all equivalent "p" orbitals are full.

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.

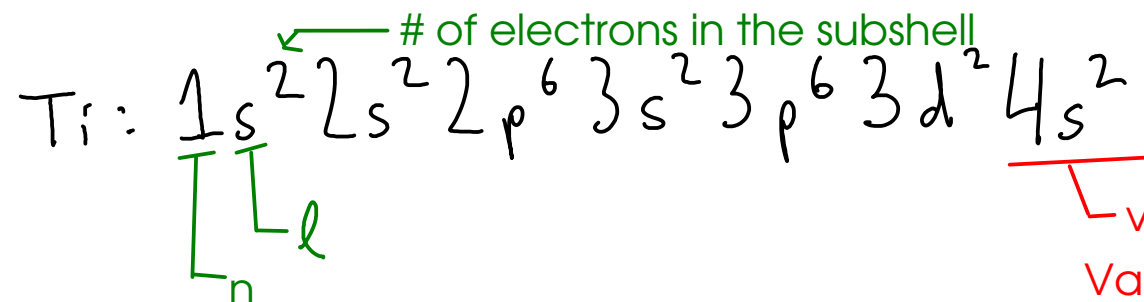
A little bit about transition metals...



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

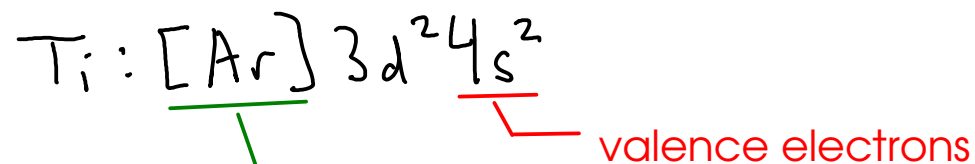
## ELECTRON CONFIGURATION (SHORT FORM)

- 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"!



"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					
IIA												VIII A					
H	He																
Li	Be											B	C	N	O	F	Ne
Na	Mg	III B	IV B	V B	VIB	VII B	VIII B	IB	IIB	Zn	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!

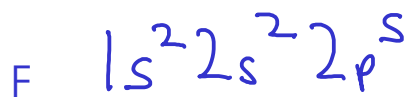
1	IA H											VIIIA He						
2	Li	IIA Be											III A B	IV A C	V A N	VI A O	VII A F	VIII A Ne
3	Na	Mg	IIIB	IVB	VB	VIB	VIIB	VIIIB	IB	IIB	Al	Si	P	S	Cl	Ar		
4	K <sub>4s</sub>	Ca	Sc <sub>3d</sub>	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga <sub>4p</sub>	Ge	As	Se	Br	Kr
5	Rb	Sr	Y <sub>4d</sub>	Zr	Nb	Mo	Tc	Ru	Rh	Pd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

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

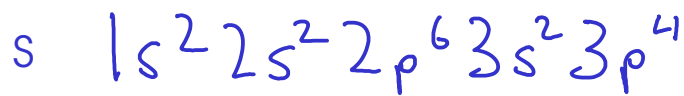
Example: Phosphorus (P):  $1s^2 2s^2 2p^6 3s^2 3p^3$

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

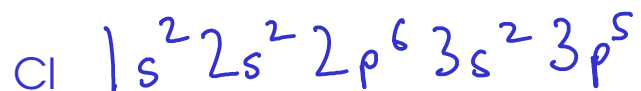
## EXAMPLES:



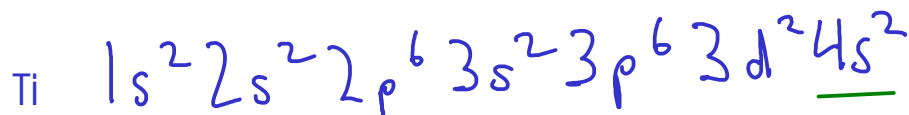
Remember - valence electrons are ALL of the electrons in the outermost SHELL (n)! More that one subshell (l) may be included in the valence electrons



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

