Chapter 8
Electron Configurations and Periodicity

I) Quantum Numbers

recap of chapter 7

A) Principle Quantum Number (n)

designates the energy level or shell of electrons

$n = 1, 2, 3, \ldots, \infty$

B) Angular Momentum Quantum Number (l)

designates the subshell

$l = 0, 1, 2, \ldots, (n-1)$

C) Magnetic Quantum Number (m_l)

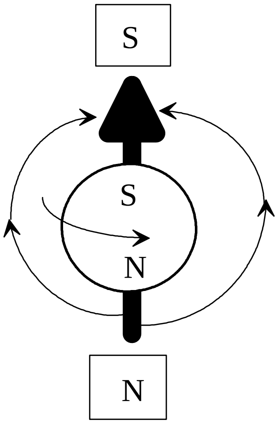
designates the orientation of the atomic orbital

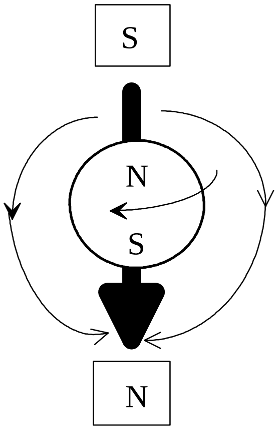
$m_l = -l \ldots 0 \ldots +l$

D) Magnetic Spin Quantum Number (m_s)

electrons rotate on an axis

e^- have a spin and can interact with a magnetic field





two orientations are possible

$m_s =$ +1/2 or –1/2

II) Electron Configurations and Orbital Diagrams

A) Electron Configurations

An electron configuration is the most stable arrangement of electrons in an atom; the ground state e^- configuration. In the ground state, the e^- are at the lowest possible energy.

example: $1s^2 2s^2 2p^1$

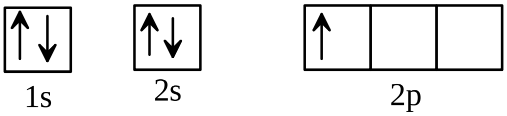
- letters represent the subshell
- numbers in front of the subshell show the shell
- superscript numbers represent the number of e^- located in that subshell

i.e. 2 e^- are located in the first shell within the *s* subshell and 2 e^- are located in the second shell within the *s* subshell and 1 e^- are located in the second shell within the *p* subshell.

B) Orbital Diagrams

Orbital diagrams (or orbital box diagrams) is a picture representation of the most stable electron arrangement in an atom. Arrows represent electrons with spin.

example:

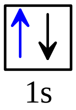


Each of the electrons in the above orbital box diagrams is represented by a set of four quantum numbers. Recall that a set of quantum numbers gives the region of space an electron may be located. Each electron in an atom has its own set of four quantum numbers

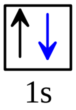
Pauli Exclusion Principle

- no two electrons in the same atom can have the same set of four quantum number.
- an orbital can hold at most two electrons which have opposite spin.

The quantum numbers for the first two electrons in the 1s subshell



$n = 1$, $l = 0$, $m_l = 0$, $m_s = +1/2$



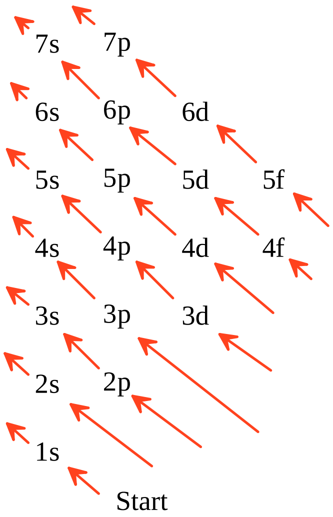
$n = 1$, $l = 0$, $m_l = 0$, $m_s = -1/2$

C) Building up principle

The electron configuration that we can predict for each element is the ground state. In the ground state, electrons exist in the lowest energy configuration.

Writing electron configurations or drawing orbital diagrams for the elements are explained by the following two rules:

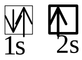
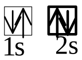
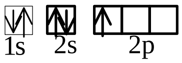
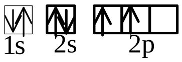
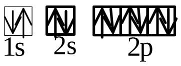
1) Aufbau Rule: Add one e^- per element to the lowest energy subshell. Successively fill subshells in the following order:
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f.



A diagram showing the build up order of subshells
start at 1s then weave back to 2s
after 2s weave back to 2p then 3s
after 3s weave back to 3p then 4s
etc.

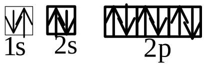
2) Hund's Rule: When orbitals of equal energy are available, the lowest arrangement with the lowest energy has the maximum number of unpaired electron with parallel spins.

example:

element	# of electrons	Orbital diagrams	e^- configuration	Quantum numbers of last e^-
H	1		$1s^1$	$n = 1, l = 0, m_l = 0, m_s = +1/2$
He	2		$1s^2$	$n = 1, l = 0, m_l = 0, m_s = -1/2$
Li	3		$1s^2 2s^1$	$n = 2, l = 0, m_l = 0, m_s = +1/2$
Be	4		$1s^2 2s^2$	$n = 2, l = 0, m_l = 0, m_s = -1/2$
B	5		$1s^2 2s^2 2p^1$	$n = 2, l = 1, m_l = -1, m_s = +1/2$
C	6		$1s^2 2s^2 2p^2$	$n = 2, l = 1, m_l = 0, m_s = +1/2$
Ne	10		$1s^2 2s^2 2p^6$	$n = 2, l = 1, m_l = +1, m_s = -1/2$

D) Noble Gas Core

The noble gas core and the pseudo-noble gas core of electrons provides an abbreviation in writing the electron configuration of an element.
The noble gas core is an inner-shell configuration corresponding to one of the Nobel gases. The pseudo-noble gas core is the noble gas core with d^{10} electrons

element	electrons	orbital diagram	electron configuration		
Ne	10		$1s^2 2s^2 2p^6$		
Na	11		$1s^2 2s^2 2p^6 3s^1$	or	$[\mathrm{Ne}]3s^1$

Examples:

Write the electron configuration for Br.

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$ or $[\mathrm{Ar}]4s^2 3d^{10} 4p^5$

Write the electron configuration for Pb.

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^2$ or $[\mathrm{Xe}]6s^2 4f^{14} 5d^{10} 6p^2$

E) Use of the Periodic Table for Electron Configurations

One can write the electron configuration for each of the elements just by looking at the periodic table.
Elements within the same group have similar electron configurations.

For example, alkaline earth metals (Group IIA)

Element	Electron Configuration		
Be	$1s^2 2s^2$	or	$[\mathrm{He}]2s^2$
Mg	$1s^2 2s^2 2p^6 3s^2$	or	$[\mathrm{Ne}]3s^2$
Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	or	$[\mathrm{Ar}]4s^2$
Sr	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2$	or	$[\mathrm{Kr}]5s^2$

Each of these elements have a noble gas core of electrons and ns^2 of electrons

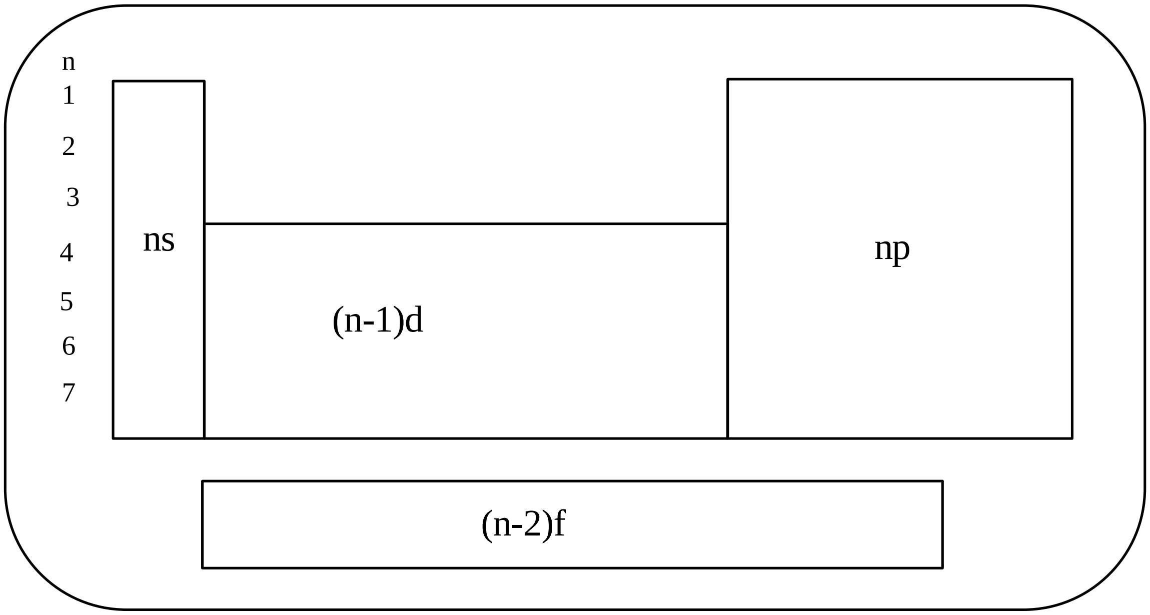
Group VA

Element	Electron Configuration		
N	$1s^2 2s^2 2p^3$	or	$[\mathrm{He}]2s^2 2p^3$
P	$1s^2 2s^2 2p^6 3s^2 3p^3$	or	$[\mathrm{Ne}]3s^2 3p^3$
As	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$	or	$[\mathrm{Ar}]4s^2 3d^{10} 4p^3$

Each of the elements have a noble gas core of e- plus ns^2np^3 electrons or $ns^2(n-1)d^{10}np^3$

The electrons outside the noble gas core of electrons are called valence electrons. The valence electrons are involved in chemical reactions and account for the similarities of chemical properties within a group of elements.

The following figure shows which subshells are filled with electrons at various points on the periodic table.

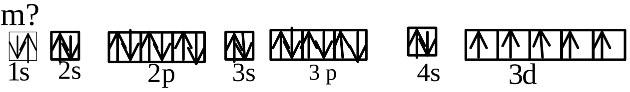


Practice:

What is the electron configuration for Ga?

What is the orbital diagram for Ti?

What is the set of four quantum numbers for the last electron in the following orbital diagram?



What is the set of four quantum numbers for the last electron in the following electron configuration? $[\mathrm{Kr}]5s^24d^{10}5p^5$

The following quantum numbers represent the last electron in an element. What is this element and give both the orbital diagram and electron configuration for this element. $n = 3$, $l = 2$, $m_l = +2$, $m_s = -1/2$

F) Exceptions to the Electron Configuration

because energies of ns & (n - 1)d sublevels are so close
some of the electron configurations do not following predictions

Conclude: Half-filled & filled sublevels are unexpectedly stable

	expect	find as more stable	
$_{24}$Cr	$[Ar]4s^2 3d^4$	$[Ar]4s^1 3d^5$	(also for Mo)
$_{29}$Cu	$[Ar]4s^2 3d^9$	$[Ar]4s^1 3d^{10}$	(also for Ag, Au)

G) Magnetic Properties of Atoms

e^- acts like small magnets
2 opposite e^- cancels out magnetic effect

Some elements are magnetic and others are not
To test put vaporized substance in magnetic field
or put solid substance which is hooked to a balance in a magnetic field.

Paramagnetic Substance
unpaired e^-
weakly attracted by magnetic field

Diamagnetic Substance [Note: ns^2, np^6, $(n-1)d^{10}$, $(n-2)f^{14}$]
only paired e^-
not attracted or repelled by magnetic field

Examples:

$_{18}$O	↑↓	↑↓	↑↓	↑	↑	(paramagnetic)
	1s	2s	2p			

$_{20}$Ca	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓		(diamagnetic)
	1s	2s		2p		3s		3p		4s		

III) Periodic Properties

Periodic Law: elements which are arranged in increasing order of atomic number vary periodically with their chemical and physical properties

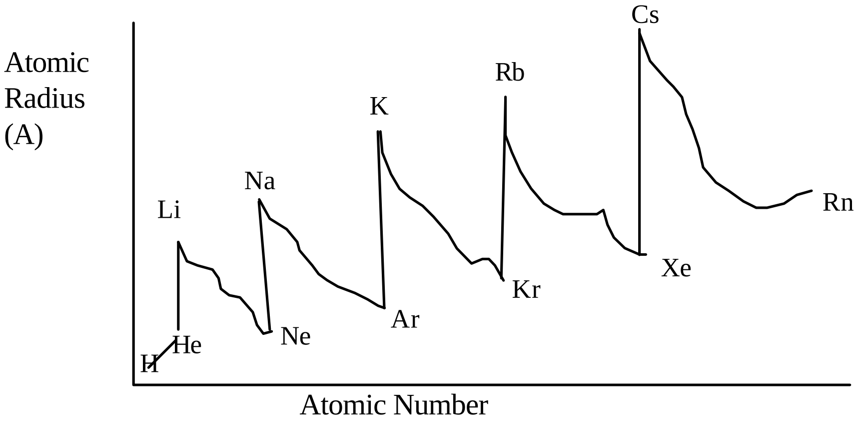
A) Atomic Radius

Recall:

- Atoms do not have definite boundaries
- electron density distribution (probability of finding an e^-) slowly drops off with increasing distance from the nucleus

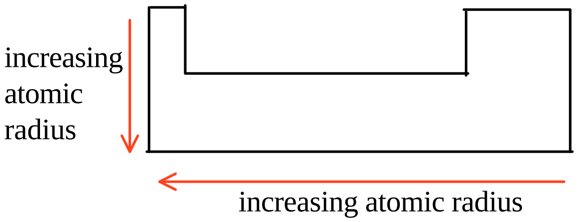
Refer to Figure 8.14 in Ebbing

the following figure is cartoon drawing for figure 8.14



Trends in the periodic table:

1) within a period: the atomic radius increase from right to left
2) within a row: the atomic radius increases from top to bottom



Factors that the atomic size variations depends on.

1) as the principle quantum number (n) increases, the atomic size increases
   reason: putting an e^- into the next higher energy level which is further from the nucleus

2) as the effective nuclear charge (Z_{eff}) increases, the atomic size decreases
   (nuclear charge actually "felt" by e^-)

reason: an e^- is placed in an energy level whose radius does not increase but the number of protons in the nucleus increase so the e^- feels a stronger attraction to positive charge an is pulled closer towards the nucleus.

Effective nuclear charge:

- the nuclear charge experienced by a particular electron in a multielectron atom, as modified by the presence of the other e^-
- the positive charge that e^- experiences from the nucleus equal to nuclear charge but reduced by shielding from other e^- in the lower energy levels

B) Ionization Energy

amount of energy needed to remove 1 mol e^- from 1 mol of gaseous atoms

1) First Ionization

minimum energy needed to remove outermost e^-

$\text{Be}(g) \rightarrow \text{Be}^+(g) + e^-$ (899 kJ/mol)

$1s^22s^2$ $1s^22s^1$

2) Second Ionization

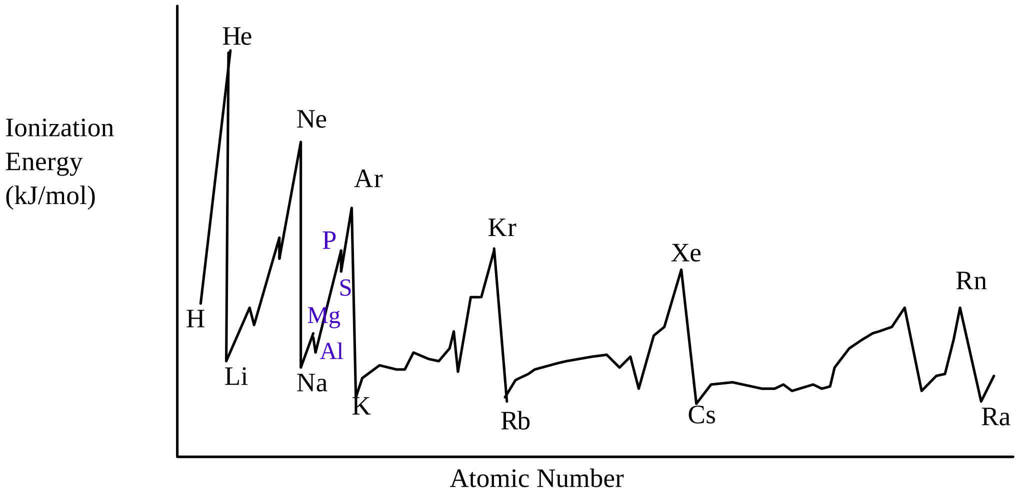
min. energy needed to remove second outermost e^-

$\text{Be}^+(g) \rightarrow \text{Be}^{2+}(g) + e^-$ (1757 kJ/mol)

$1s^22s^1$ $1s^2$

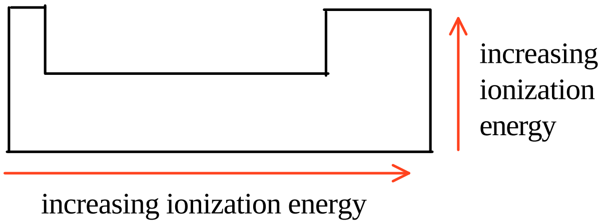
Refer to Figure 8.17 in Ebbing

the following figure is cartoon drawing for figure 8.17



Trends in Ionization Energy

1) within a period (left to right): ionization energy increases with an increase in atomic number
2) within a group (bottom to top): ionization energy increases with a decrease in atomic number



Energy needed to remove e^- from the outershell depends on

1) effective nuclear charge
2) average distance of e^- from the nucleus

(i.e.) when the effective nuclear charge increases or distance from the nucleus decreases the attraction between the e^- and the nucleus increases, therefore increasing the ionization energy.

Exceptions:
Why is there a decrease in the ionization energy between P and S or Mg and Al?
It is easier to remove an e from an orbital that is not half filled or completely filled, than one that is.

Refer to Table 8.3 in Ebbing

TABLE OF IONIZATION ENERGIES shows:

- Successive removal of e^- requires more energy Why? After the first e^- is removed, the successive e^- are being removed from a positive ion, which strongly attracts an e^-.
- Once the noble gas configuration is achieved the ionization energy of the element sky rockets. Why? It requires much energy to remove an e^- from a completely filled shell.

C) Electron Affinity

Energy change that occurs when an e$^-$ is added to a gaseous atom or ion

$$\underset{1s^22s^22p^5}{\mathrm{F}} + 1\,\mathrm{e}^- \rightarrow \underset{1s^22s^22p^6}{\mathrm{F}^-}$$

Energy is evolved when e$^-$ is added, therefore electron affinity values have a negative sign (more negative electron affinities have the greater attraction for an e$^-$)

refer to Table 8.4 for electron affinities of the main group elements in Ebbing

Trends

1) within a period (left to right), the electron affinities become more negative
2) within a group (top to bottom), the electron affinities do not change greatly

D) Electronegativity Values

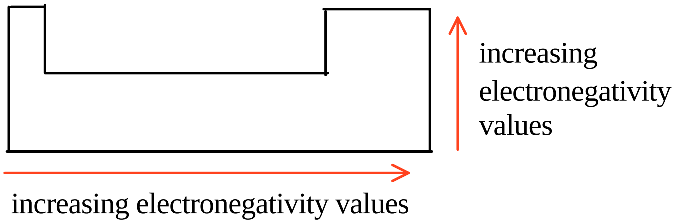
ability for an atom to attract e$^-$ to itself (e$^-$ pulling power)

Electronegativity scale used was developed by Linus Pauling

refer to Table 9.11 for Electonegativies in Ebbing

Trends

1) within a period (left to right), the electronegativity values increase.
2) within a group (bottom to top), the electronegativity values increase.



E) Ionic Radii (Sizes of Ions)

The size of an ion depends on:

1) nuclear charge
2) number of e^- it possesses
3) orbitals in which outer-shell e^- reside

Positive ions (Cations)

- formed by removing e^- from outermost shell
- decreases total e^-/e^- repulsion
- vacates most spatially extended orbital

therefore, a cation is smaller than its parent atom

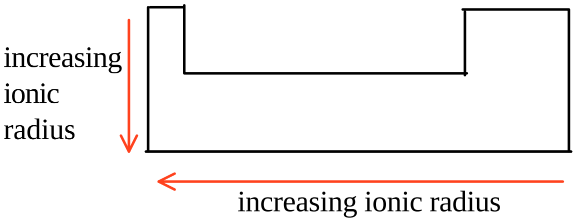
Negative ions (Anions)

- formed by adding e^- to outermost shell
- increases e^-/e^- repulsions
- causes e^- to spread out more in space

therefor, an anion is larger than its parent atom

Trends

1) within a group (top to bottom), ions of same charge increase in size going down a group
2) within a period, ions increase in size from right to left.



Isoelectronic series: ions possessing the same number of e^-

ionic radius of ions in an isoelectronic series decrease with an increase in nuclear charge (same number of e^-; but larger number of p^+)

The following isoelectronic series is in order of decreasing ionic radius.

$O^{2-} > F^- > Na^+ > Mg^{2+} > Al^{3+}$

all of the above ions have 10 e^-

and an electronic configuration for Ne: $1s^22s^22p^6$

IV) Brief Descriptions of the Main-Group Elements

READ SECTION 8.7 in Ebbing on your own