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Unit 7

Advanced Topics in Atomic Structure & Periodic Table

- Compare the properties of the isotopes of an element.
- Distinguish between a *continuous spectrum* and a *line spectrum*.
- Explain how the lines in the emission spectrum of hydrogen are related to electron energy levels.
- Deduce the electron arrangement for atoms and ions up to Z = 20.
- Define the terms first ionization energy and electronegativity.
- Describe and explain the trends in atomic radii, ionic radii, first ionization energies, electronegativities and melting points for the alkali metals and the halogens.
- Describe and explain the trends in atomic radii, ionic radii, first ionization energies and electronegativities for elements across period 3.
- Compare the relative electronegativity values of two or more elements based on their positions in the periodic table.
- Discuss the similarities and differences in the chemical properties of elements in the same group.
- Discuss the changes in nature, from ionic to covalent and from basic to acidic, of the oxides across period 3.

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Electron Configuration

Rules of the filling of orbitals: (How to determine the arrangement of electrons.)

1. **Aufbau Principle:** electrons occupy the orbitals of lowest energy first. in other words, a "1s" gets filled before a "2s", which in turn gets filled before a "2p".
2. **Pauli Exclusion Principle:** A single atomic orbital contains, at most, two electrons (opposite spins).
3. **Hund's Rule:** Orbitals of equal energy (for example 3 p's or 5 d's) are filled one electron at a time (all are negative, so they repel). They don't want to be in the same space if they don't have to.

Watch the "Orbitals" PowerPoint on the class web site now!! (it will help tremendously with understanding the material)

ELECTRON CONFIGURATIONS OF THE ELEMENTS

- Look at Table 5.3, page 134, and the table to the right to figure out the progression for filling orbitals. Remember the rules!
- Filling orbitals up to Element 18 (Argon) follows a logical sequence. But when we get to potassium (K), something strange occurs. We fill 4s before we fill 3d. This is because principle energy levels 3 and 4 overlap and 4s is lower in energy than 3d.
- **Read page 133-135 in your textbook. Using that information and the table to the right, write the electron configuration for each atom below:**

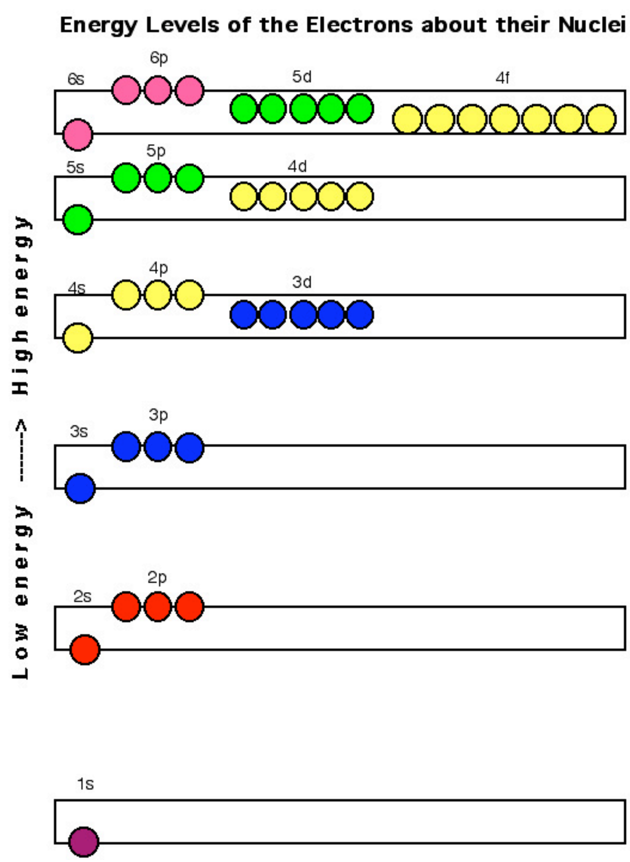
Carbon: ________________________________

Argon: ________________________________

Nickel: ________________________________

Boron: ________________________________

Silicon: ________________________________



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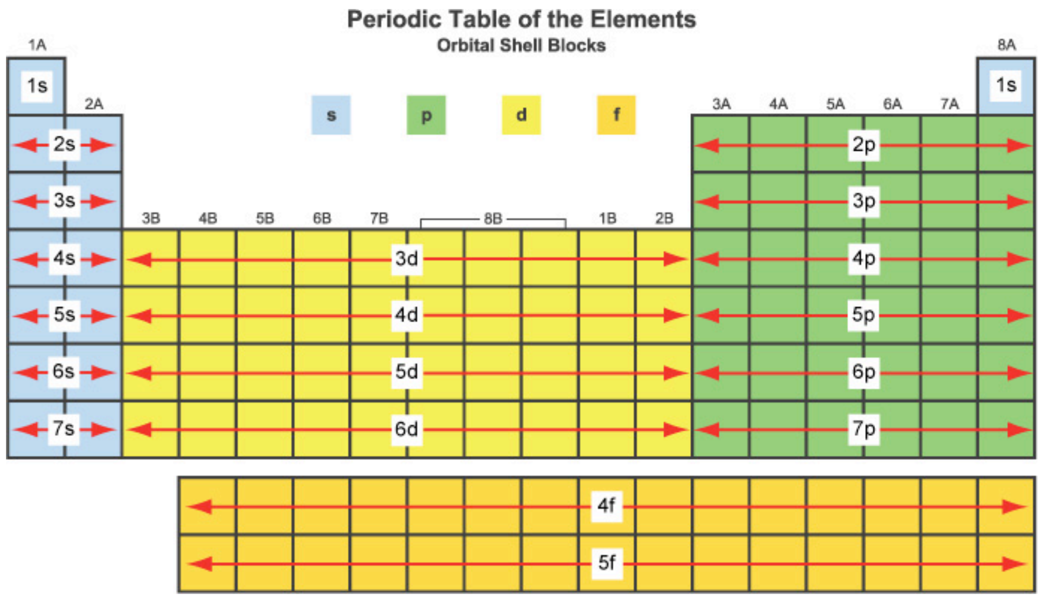
Electron Configuration and The Periodic Table

Now, let's connect this information to the periodic table. (If you had trouble with the previous page, this may help) Read p. 166 in your textbook – the section titled "Blocks of Elements" and examine the periodic table below.

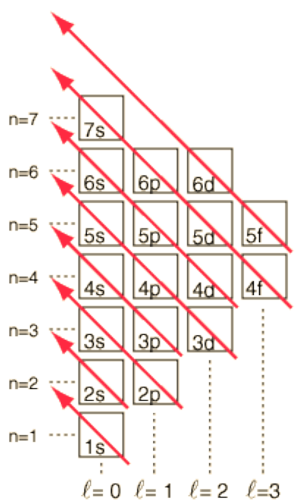


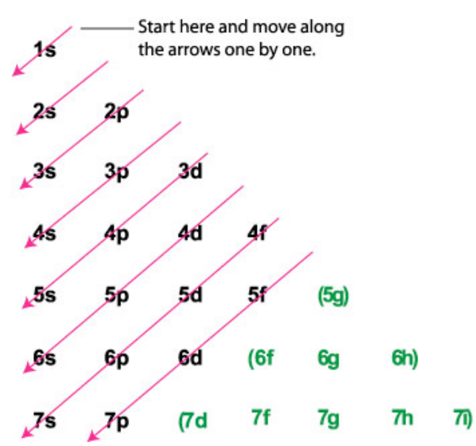
You can use this pattern on the periodic table to help you determine the electron configuration of an element. As you increase in atomic number (and hence # of electrons), you enter these orbital shell **BLOCKS**, identified with ***s, p, d, or f.***

Try it! Use the periodic table "blocks" to help you write the electron configuration of these elements:

Chlorine: ________________________________ **Vanadium:** ________________________________

Barium: ________________________________ **Krypton:** ________________________________





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Location of Electrons

Electrons are in regions of the atom known as orbitals. Roughly speaking, they are located in principal energy levels similar to the shells or energy levels of the Bohr model. Each of the energy levels is designated by a quantum number, *n*, from 1 to 7. None of the known elements has atoms with more than 7 principal energy levels. The principal energy level with the lowest energy is 1. The highest is 7. Principal energy levels can be thought of as being subdivided into energy sublevels. The maximum number of sublevels in a principal energy level is *n*, but none of the existing elements use more than 4 sub levels even in principal energy levels 5-7. Sublevels are designated by the letters s, p, d, and f, in increasing order of energy. The orbitals are regions within a sublevel where electrons of a given energy are likely to be found. There are a maximum of 2 electrons in an orbital. A useful analogy to help you visualize this is an apartment building. Each apartment represents a sub level. Each bedroom represents an orbital. The electrons are the tenants in the bedrooms. Electrons are most likely to be found in the lowest energy locations available. Knowing this, it is possible to figure out how the electrons are arranged in an atom.

The number of orbitals within a sub level varies in a predictable pattern. The number of orbitals within a sub level and the maximum number of electrons is as follows:

Sublevel	**s**	**p**	**d**	**f**
Number of orbitals	1	3	5	7
Maximum Number of Electrons	2	6	10	14

The first energy level has only one sublevel, s; the second energy level has to sub levels, s and p; the third energy level has three sub levels, s, p, and d; and so on This results in the pattern shown below:

Principal Quantum Number (n)	**Number of Orbitals (n^2)**	**Orbitals per Sublevel**				**Maximum Number of Electrons ($2n^2$)**
		s	**p**	**d**	**f**	
1	1	1	-	-	-	2
2	4	1	3	-	-	8
3	9	1	3	5	-	18
4	16	1	3	5	7	32

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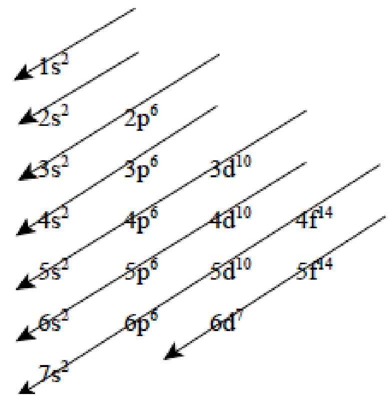
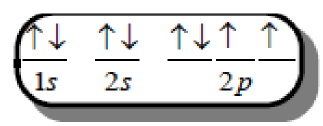
The electrons are arranged according to the following rules:



1. the number of electrons equals the number of protons (atomic number).
2. electrons occupy orbitals in sequence beginning with those of the lowest energy (see diagram).
3. in a given sublevel, a second electron is not added to an orbital until each orbital in the sublevel contains one electron.

This results in the order of filling for elements 1 to 109 pictured below. Follow each arrow from beginning to end. Then go to the beginning of the next arrow down. When you follow this pattern, you will note that no more than four orbitals are occupied in the outermost principal energy level. This is because once the p sub-level is filled, the next energy sub-level is always the s in the next principal energy level. Oxygen has 8 protons and 8 electrons. Its electron configuration in ***sub-level notation*** is as follows: $1s^22s^22p^4$. This means there are 2 electrons in the first level and 6 in the second (add the superscripts). As a result the electron arrangement can also be written as follows: 2-6. This is known as the ***Bohr notation***.

Remember, electrons never pair in an orbital until every orbital in a sub-level has an electron. When they do pair, they spin in opposite directions. This reduces the repulsion between them. The opposite spins of the electrons are represented by up arrows and down arrows. The electron configuration of oxygen can be depicted as follows:



Each horizontal line represents an orbital in a sub-level. Each arrow represents an electron in an orbital. This is called ***orbital notation***.

For each of the elements below, write the sub-level, Bohr, and orbital notation.

Element	**Atomic Number**	**Electron Configurations**		
		Sublevel Notation	**Bohr Notation**	**Orbital Notation**
H	1			
N	7			
Ca	20			
Al	13			
Cu	29			
C	6			
Ar	18			

Name: ________________________________-

Chemical Properties Based on Electron Configuration

You already know that chemical properties of elements are determined by their electron configuration and valence electrons. Let's look more closely at the similarities in electron configuration.

- Note that the similar chemical properties of Na and K are consistent with similar electron structure:

Na: $1s^2 2s^2 2p^6 3s^1$ K: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

- Likewise, Mg and Ca are similar in structure and similar in reactivity and properties:

Mg: $1s^2 2s^2 2p^6 3s^2$ Ca: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

- when we get to scandium (atomic #=21), the 3d orbitals get filled one electron at a time in one orbital until they are 1/2 filled and then we go back and add one electron at a time until the orbitals are completely filled.
- Now we are at **Ga ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$)**

- Group 1 elements have similar chemical properties because all can lose 1 electron to form a **filled shell or filled p sub-shell**.

Li ($1s^2 2s^1$) $- 1e^- \rightarrow$ Li^+ ($1s^2$)

Na ($1s^2 2s^2 2p^6 3s^1$) $-1e^- \rightarrow$ Na^+ ($1s^2 2s^2 2p^6$)

K ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$) $-1e^- \rightarrow$ K^+ ($1s^2 2s^2 2p^6 3s^2 3p^6$)

Rb ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1$) $-1e^- \rightarrow$ K^+ ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$)

- All Group 17 elements have similar chemical properties because all can gain 1 electron to form a **filled shell or filled p sub-shell**.

Cl ($1s^2 2s^2 2p^6 3s^2 3p^5$) +1e- $\rightarrow$ Cl^- ($1s^2 2s^2 2p^6 3s^2 3p^6$)

Br ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$) +1e- $\rightarrow$ Br^- ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$)

Name: ________________________________-

Those Wacky Transition Metals

- The 10 elements that use the five 3d orbitals (capacity = 10 electrons) are called TRANSITION ELEMENTS or TRANSITION METALS (because they are all metals).

- What about the transition elements? These metals often have multiple valences (that is, they can lose difference numbers of electrons because of the stability of configurations involving d-electrons.) One consideration is that 1/2 filled sub-shells have a unique stability. that is d^5 is more stable than d^4 or d^6. Also, s electrons are usually removed in preference to d electrons.

- Iron (Fe) (atomic #=26) atoms have a configuration of $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

- Iron will lose 2 electrons to become $Fe^{2+} = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^6$

- OR lose 3 electrons to become $Fe^{3+} = 1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^5$

- There are lots of other examples, BUT please keep in mind explanations like the one above come after experimental data is obtained! So, if you know that oxides of iron have the formulas FeO and Fe_2O_3, an explanation based on electron structure can be given. *As long as this explanation can be tested and can be used to predict other results, it is valid science!*

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More About - Periodic Trends

• Many chemical and physical property trends in the Periodic Table can be explained by **COULOMB's LAW**:

$$F = \frac{k\, Q_1 Q_2}{r^2}$$

This says that the force of attraction or repulsion (F) between 2 particles is dependent on the product of the charges of the particles (Q_1 and Q_2) divided by the distance between the two particles (r) squared.
(k is a constant dependent on the nature of the particles)

We need to consider a number of quantites related to atoms of elements:

1. Size of the atom (the radius - from center of nucleus to outer electron shell)

2. Nuclear charge (the number of protons in the nucleus)

3. Shielding (number of "inner" electrons, NOT valence electrons)

4. Effective nuclear charge (nuclear charge – shielding)

Let's look at 3 metals, make some "observations" based on structure, and draw some conclusions about trends based on Coulomb's Law.

Na	Mg
K	

1. Size of atoms:

- K is bigger than Na because K has 4 shells and Na has only 3
- Na and Mg ?????? We need to consider Coulomb's Law

2. Nuclear charge:

+11	+12
+19	

3. Shielding:
(inner electrons)

-10	-10
-18	

4. Effective Nuclear Charge:
(#2 - #3)

+1	+2
+1	

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Now, let's consider **trends:**

1. **Size:**
   1. As you down a group, size increases due to extra shells or orbits.
   2. As you go across a period, size decreases because the effective nuclear charge increases and according to Coulomb's Law, that would make the force of attraction between the nucleus and the outer electrons greater. This would result in a **decrease in size ad the effective nuclear charge increases.**

2. **Ionization energy (energy required to remove an electron):**
   1. As you go down a group, the distance between the + nucleus and the – valence electrons increase, resulting in a decrease in attraction and easier removal of an electron.
   2. As you go across a period, the attraction between positive nucleus and valence electrons increase due to a more effective nuclear charge (Coulomb's Law). this means it's more difficult to remove an electron as you go across the Table (from Groups 1-18 in the same period).

3. **Electronegativity (attraction of electrons):**
   1. Same arguments as in 2 (above)! Down a group, electronegativity decreases.
   2. Same arguments as in 2 (above)! Across a period, electronegativity increases.

Answer the following questions:

1. Why is the 1st ionization energy of Na smaller than the 1st ionization energy of Mg, but the 2nd ionization energy of Na is much larger than that of Mg? ____________________________
   ____
   ____
   ____
   ____

2. Which metal is the most reactive? (Explain in terms of ease of losing an electron and Coulomb's Law). ____
   ____
   ____
   ____

3. Which element has the highest electronegativity? Explain in terms of attraction of electrons and Coulomb's Law. ____
   ____
   ____
   ____

Name: ________________________________-

Assignment: Review

Answer the following questions. Refer to your text book and internet resources as needed for help.

1. Identify which group on the periodic table each electron configuration should be found in.
   - A) $[Ne]3s^2 3p^5$ ______________________
   - B) $[Ar]3d^{10} 4s^2 4p^2$ ______________________
   - C) $[Ne]3s^2$ ______________________
   - D) $[Ar]4s^2 3d^{10} 4p^1$ ______________________
   - E) $[Xe]4f^{14} 5d^4 6s^2$ ______________________

2. Based strictly on position on the periodic table, give the number of
   - A) outer energy level electrons in an atom of Sb ___________________
   - B) electrons in n = 4 atoms of Pt ______________________
   - C) elements with six valence electrons _________________
   - D) transition elements in the 6th period _________________

3. Write the likely electron configurations for the following ions:
   1. Mn^{+6} ______________________________________
   2. Co^{+2} ______________________________________

4. Define *isoelectronic*: ____

   ____

   ____

5. Of the following isoelectronic species, explain which will have the smallest radius, using Coulomb's Law reasoning: the cesium ion or the iodide ion

   ____

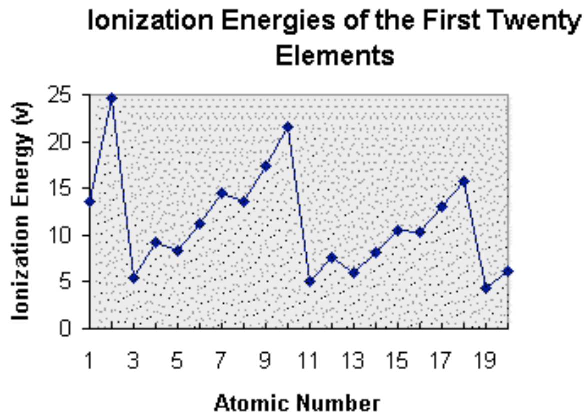
   ____

   ____

   ____

Name: ______________________________-

6. As one crosses the periodic table to the right in a given period, the ionization energies are expected to trend upward. However, as shown on the graph below, the trend is not smooth. Notice the spikes at the elements with s^2 and also with p^3 positions.



A) How do you explain the spike at s^2? (Hint: Think about He.)

B) How do you explain the spike at p^3? (Hint: What about p^3 that results in especially great stability, and why does ionization energy increase as a result??)

7. How would you expect the radius of H^- ion to compare with that of He atom? Use Coulomb's Law to explain.

8. Explain why…
A) The 2nd ionization energy is usually higher than the 1st ionization energy for elements.

B) The opposite is true for an element like calcium.

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14. The configuration Cr differs from that derived by the Aufbau procedure. (See text p. 136 for help)

(A) Write the *expected* configuration ___________________________

(B) Write the actual configuration ___________________________

(C) Explain the actual configuration in terms of stability.

15. Arrange the following groups in order of
1 – increasing ionization energy
2 – increasing electronegativity

A) N, B, F, Ne

B) Mg, Ca, Sr, Ba, Hg