Review of energy levels (atomic orbitals)

The energy levels for electrons in atoms are called atomic orbitals:

1. Quantized (discrete) energy levels.

2. The electron is a three-dimensional wave-particle that is delocalized over space without an exact location or exact motion. Fig. 7.10, Figs. 7.13-7.15.

3. The periodic table lists atomic orbitals in order from lowest to highest energy.

Bound electrons are delocalized in quantized energy levels that are three-dimensional.

Mathematically, we can calculate the energy of the atomic orbitals (i.e., energy of the levels):

$$E_n = -\frac{2\pi^2 m e^4 Z^2}{(4\pi\varepsilon_o)^2 h^2} \times \frac{1}{n^2}$$

n = 1 is the first level (the ground state)

n = 2 is the second level (the first excited state, 1 level above the ground state)

n = 3 is the third level (the second excited state, 2 levels above the ground state)

This equation and variations of this equation are only correct for hydrogen and hydrogen-like ions (ions with only 1 electron).
Examples: H, He^+, Li^{2+}, etc.

More complicated equations are needed for other situations.

Most often the equation is used to calculate ΔE for the electronic transitions in H-like atoms.

$$\Delta E = -2.179 \times 10^{-18}\ \text{J} \left(\frac{1}{n^2_f} - \frac{1}{n^2_i} \right) = h\nu$$

<u>Example</u>:
Calculate the energy for the n = 3 to n = 2 transition in a hydrogen atom.

Some variations of this equation replace ΔE with ν_{photon} or $1/\lambda_{photon}$.

Atomic Orbitals and Quantum Numbers

Representations of atomic orbitals: s, p, and d orbitals (Fig. 7.15). Also, http://library.thinkquest.org/3659/structures/shapes.html

These pictures describe electron density, the region of space where the electron is likely to be found (Figs. 7.13 and 7.10).

They show the outer surface of the region that the electron occupies with 90% probability.

Orbitals are also called <u>wave functions</u>, a mathematical function that most correctly describes the region of space occupied by an electron.

Note that there are <u>nodes</u>, areas of zero electron density (0% probability of finding the electron).

We use quantum numbers to name the energy levels (the orbitals).

n: principal quantum number, gives the energy, gives the size, shell, row.

n must be a positive integer (n = 1, 2, 3, …).

Larger *n* means the electron has more energy and occupies a larger region of space, i.e., the electron is in a larger orbital.

l: azimuthal quantum number, gives the shape.

l is restricted by *n*, can be zero or a positive integer less than *n* (l = 0, 1, 2, …, n-1).

l	orbital / shape / location in the periodic table
0	s / sphere, 1 lobe, 0 nodes / left
1	p / 2 lobes, 1 node / right
2	d / 4 lobes, 2 nodes / middle

$\underline{m_l}$: “m sub l”, magnetic quantum number, specifies an orbital, gives orientation of the orbital, gives direction.

$\underline{m_l}$ is restricted by l, can be any integer between $-l$ and $+l$, including zero.
$m_l = -l, \ldots, 0, \ldots, +l$ (or, $m_l = 0, \pm 1, \pm 2, \ldots, \pm l$)

$\underline{m_s}$: “m sub s”, spin orientation quantum number, spin, gives orientation of the electron, “up” or “down”.

$\underline{m_s}$ can be +1/2 or -1/2.

Electrons have a property called “spin” that can only have values of ±1/2. The electron is not literally spinning, but this is the name given for this property (Fig. 7.12).

With 3 quantum numbers (n, l, m_l) we can label every atomic orbital (picture analogy p. 242).

With all 4 quantum numbers, we can give a unique label to every electron in every atom (picture analogy p. 242, Pauli exclusion principle).

<u>Examples</u>:
H: 1s orbital (n=1, l=0, m_l=0) and m_s= +1/2
He: 1s orbital and m_s= +1/2
1s orbital and m_s= -1/2

Orbital box diagrams

H:

He:

Electron configurations

Electron configuration notation ($1s^1$, $1s^2$, etc.)
H: $1s^1$ = 1 e^- in the 1s orbital.

He: $1s^2$ = 2 e^- in the 1s orbital.

1. Each e^- is labeled by a unique set of 4 quantum numbers. (Pauli exclusion principle: one atomic orbital can hold at most two electrons, but only if the two electrons have opposite spins.)

2. The periodic table shows the order of orbital energies and the s, p, d, and f blocks.
1s is the lowest energy orbital.

3. Electron configurations of any atom can be built up (aufbau) by starting from the 1s orbital.
B:

C:

N:

O:

*Some orbitals have the same energy (called <u>degenerate orbitals</u>)

*Electrons repel each other => avoid pairing electrons, try for maximum spin (Hund's rule).

Practice: For the element Ti ($Z = 22$), write the electronic configuration and draw the orbital box diagram.

Core and valence electrons

Core electrons are generally not reactive.
Valence electrons are reactive (Chapter 8).

Core electrons: electrons at lower energy, electrons that fill an inner shell (fill a row), inner electrons.

Valence electrons: electrons at higher energy, electrons in an unfilled shell (unfilled row), outer electrons.

C: $1s^2 2s^2 2p^2$

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

Noble gas abbreviation = core electrons

C:

Na:

<u>Practice</u>: For the element Ti (Z = 22), write the electronic configuration using the noble gas abbreviation.

Identify the valence and core electrons.

Give the quantum numbers for the valence orbitals and electrons.
(hint:
$n = 1, 2, 3, \ldots$
$l = 0, 1, 2, \ldots, n-1$
$m_l = -l, \ldots, 0, \ldots, +l$
$m_s = +1/2$ or $-1/2$)

Electron clouds

Electrons surround the nucleus of an atom and form an electron cloud.

A collision between atoms is a collision between their electron clouds.

The clouds repel each other (the atoms bounce off each other) because electrons are negative. Examples: hitting a table, gas particle collisions cause pressure.

At the same time, the negative cloud of one atom is attracted to the positive nucleus of the other atom.

So atoms can come close to each other. Examples: condensation from gas to liquid, freezing from liquid into solid.

Sometimes atoms come close enough to react with each other if they have enough energy. Example: any chemical reaction.

The interaction between the electron clouds, like sharing clouds between atoms, is fundamental to chemical properties of atoms and compounds.

Chapters 7, 8, and 9 start examining electrons and the resulting chemical properties of atoms.