Atomic Theory

A **tested explanation** of the atom.

Review:

•From Thomson's experiment with CRTs we know that atoms have electrons that have a negative charge.

•From the gold foil experiment we know that atoms have a nucleus that is very small (less than 0.001% of the volume) and is most (more than 99.999%) of the mass.

Atomic Theory

- From x-ray experiments and others we know that the nucleus of the atom contains positively charged protons and neutral neutrons.
- We know the mass, charge and position of protons and neutrons, we know the mass and charge of electrons.

What we don't know - We need an explanation.

Where are the electrons?

Why do they occupy so much space?

What is the function of the electrons in the atom?

Atomic Theory

The first proposal of what the electrons are doing came from Rutherford.

Rutherford suggested that the electrons might just be "floating" near the nucleus. This has some important problems, most importantly that the opposite charge of the electrons and the protons should mean that floating electrons would be pulled into the nucleus. The atom then wouldn't exist.

The Bohr Model

A second possible explanation by Rutherford suggested that the electrons might travel in orbits around the nucleus much like the planets around the sun. This proposal had the same problem, the electrons should very quickly crash into the nucleus.

Niels Bohr began working with Rutherford and proposed a possible solution to this problem. Bohr suggested that electrons should only be allowed to travel in certain well defined orbits.

The Bohr Model

Bohr had some evidence for this, measurements of light being emitted from single elements showed a pattern of bright lines that are well defined, not a continuous spectrum that would be predicted if the electrons could be in any position around the atom.

Since the elements only gave off a few, well defined colors, the electrons could only be in a few, well defined locations. These locations became the defined orbits for Bohr.

The Bohr Model

Spectral Emission Lines

http://astro.u-strasbg.fr/~koppen/discharge/discharge.html

Wave Particle Duality

The Bohr model worked well for hydrogen and helium but when the atoms got more complicated (more electrons) the model didn't work very well.

Many discoveries were made around this time that increased the complexity of the picture of the atom. One of these suggested that light might not be a wave at all but instead a particle. Since light had properties of both a wave and a particle the idea of wave particle duality was introduced.

Wave Particle Duality

If light had properties of both waves and particles maybe other things did as well. One of the first to be tested were electrons. Electrons have mass, they have a charge, they bounce off other objects. In every sense they show properties of being a particle.

In a classic test, a beam of electrons was directed at a barrier that had two slits. The result was that the electrons behaved like waves. The electrons went through both slits at the same time.

Wave Mechanics

Erwin Schrodinger used data from Bohr and others (the same kind of data you collected with the different colors of light from single elements) to put together an equation to predict the positions of electrons.

The equation that worked has a combination of wave principles and probability.

The equation is complicated but it works. The equation has 4 variables (not just 2 like "normal" math equations of x and y).

The Schrodinger Equation

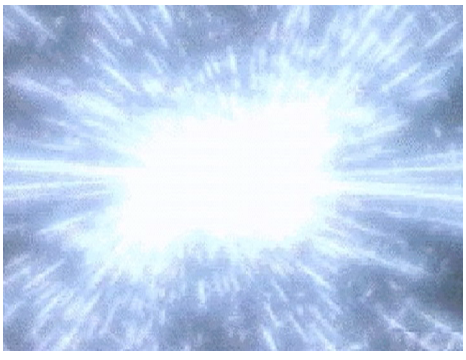
Quantum Chemistry

Quantum Numbers

The four different variables in the Schrodinger equation are called quantum numbers.

The name comes from the idea that electrons make quantum jumps (or leaps) from one position to the next. There is a minimum change in position of the electrons.

Quantum Leap TV Show



Quantum Numbers

The four quantum numbers are given the symbols of

n

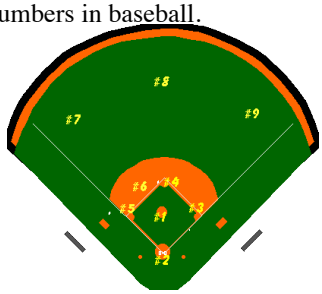
l

m_l

m_s

Electron positions

These quantum numbers tell us the probable (approximate) positions of the electrons just like position numbers in baseball.



n - the principal quantum number

The first quantum number - n is called the principal quantum number because it describes the biggest part of the energy relationship of the electron.

In chemistry we often refer to this quantum number as the energy level.

n has possible values of the whole numbers (1, 2, 3 ….)

l - the orbital shape quantum number

The second quantum number - l is called the orbital shape quantum number because it describess the shape of the orbital in the Schrodinger equations.

In chemistry we often refer to this quantum number as the sublevel.

l has possible values of 0, 1, …., n-1

This means that if n=1 the only possible value for *l* is 0

If n=2, l can be either 0 or 1

m_l - magnetic orientation quantum number

The third quantum number - m_l is called the magnetic orientation quantum number. It describes the position of the orbitals in a magnetic field.

In chemistry we often refer to this quantum number as the orbital.

m_l has possible values of $-l, \ldots, 0, \ldots +l$

This means that if l=0, m_l is 0

If l=1 then m_l can be -1, 0, or +1

If l=2 then m_l can be -2, -1, 0, +1, +2

m_s - magnetic spin quantum number

m_s is the magnetic spin quantum number.

We have no evidence to indicate electrons are spinning.

We cannot see individual electrons. We don't know what shape they have (even though we often draw them as balls).

Electrons do exhibit a property that in physics is called angular momentum. Macroscopic objects that have angular momentum are spinning so we describe electrons in the same way.

m_s - magnetic spin quantum number

m_s has possible values of -½and +½.

We usually represent this in chemistry with either an up or a down arrow. ↑↓

Orbital "Pictures"

It is possible to graph the Schrodinger equations much like you would graph a line from the equation y=mx + b.

The graphs of these equations match very well to experimental measurements of where we find the electrons in the atom.

The correlation of the graphs with the actual measurements is one of the reasons why the quantum mechanical model is the current model of the atom for chemistry.

Graphical representations of orbitals

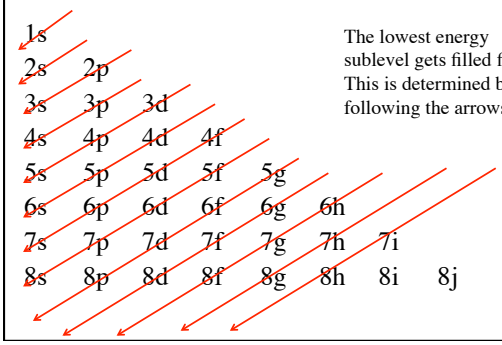
Rules Simplified

Quantum numbers simplified to energy levels, energy sublevels, orbitals and "spin".

1s						
2s	2p					
3s	3p	3d				
4s	4p	4d	4f			
5s	5p	5d	5f	5g		
6s	6p	6d	6f	6g	6h	
7s	7p	7d	7f	7g	7h	7i

notice that the number of sublevels (s, p, d, f, etc) matches the energy level

Rules Simplified



The lowest energy sublevel gets filled first. This is determined by following the arrows.

Rules Simplified

s sublevel has one orbital
p sublevel has three orbitals
d sublevel has five orbitals
f sublevel has seven orbitals

s __
p __ __ __
d __ __ __ __ __
f __ __ __ __ __ __ __

Each sublevel has orbitals represented by blanks (or circles or boxes).

Rules Simplified

↓↑

Each orbital can "hold" at most two electrons and they must have opposite spin (Pauli Exclusion Principal).

sodium

sodium has 11 p^+ and 11 e^-

1s↓↑ 2s↓↑ 2p↓↑ ↓↑ ↓↑ 3s↓_

chlorine

chlorine has 17 p^+ and 17 e^-

1s↓↑ 2s↓↑ 2p↓↑ ↓↑ ↓↑ 3s↓↑ 3p↓↑ ↓↑ ↑

When there are multiple orbitals in a sub level, each orbital gets one electron before any get two.