## 5. Quantum Mechanical Model of the Atom

ψ, (y, Psi)describes the wave function (orbital). Schrodinger's Wave Equation: A specific wave function (for all the possible solutions) is called an **orbital**. The electron occupies a *probable* (Heisenberg Uncertainty Theory; a particles exact momentum and position can not be known at the same time) region in space called an orbital, not an orbit. This uncertainty is so small for larger objects that it is unnoticed. $\Psi^2$ is the probability distribution. An orbital = electron density map.

***The size of the H 1s orbital is the radius of a sphere that encloses 90% of the total electron probability.***

## 6. Quantum Numbers

Solutions of Shrodinger's Equation give more than one wave function: Quantum Numbers

1.) **The Principal Quantum Number**, (n): "shell", Related to size and energy of the orbital larger value of n means larger size and greater energy. Ex. N=1, 2, 3, …

2.) **Azimuthal Quantum Number, Angular Momentum(l):** "sublevel", 0 through n-1 for each value of n. Describes shape of atomic orbital. Letters accompany these numbers. Ex. n=3 can have 0 to n-1 where n=3, therefore 0, 1, and 2 such that 0=s (3s), 1 = p (3p) and 2=d (3d).

3.) **Magnetic Quantum Number, ($m_\ell$):** Describes orientation of orbital in space. Has values of $\ell$ and –$\ell$. For example: If $\ell$ = 1 (p sublevel), then –1, 0, 1 exist. Describes the x,y,z orientation of the orbitals.

**Table 7.1** The Angular Momentum Quantum Numbers and Corresponding Letters Used to Designate Atomic Orbitals

| Value of $\ell$ | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| Letter Used | *s* | *p* | *d* | *f* | *g* |

**Table 7.2** Quantum Numbers for the First Four Levels of Orbitals in the Hydrogen Atom

| *n* | $\ell$ | Orbital Designation | $m_\ell$ | Number of Orbitals |
|---|---|---|---|---|
| 1 | 0 | 1*s* | 0 | 1 |
| 2 | 0 | 2*s* | 0 | 1 |
| | 1 | 2*p* | −1, 0, +1 | 3 |
| 3 | 0 | 3*s* | 0 | 1 |
| | 1 | 3*p* | −1, 0, 1 | 3 |
| | 2 | 3*d* | −2, −1, 0, 1, 2 | 5 |
| 4 | 0 | 4*s* | 0 | 1 |
| | 1 | 4*p* | −1, 0, 1 | 3 |
| | 2 | 4*d* | −2, −1, 0, 1, 2 | 5 |
| | 3 | 4*f* | −3, −2, −1, 0, 1, 2, 3 | 7 |

## 7. Orbital Shapes and Energies

Nodal surface (nodes); region of zero probability of finding an electron.

Shapes of orbitals on pages 307 – 309. Note shapes and orientation. s is spherical, p are dumbbell, d and f are more complex.

**Degenerate Orbitals**: Orbitals with the same energy. All of the atomic orbitals are available to H's electron, but the ground state, 1s, is the lowest energy state.

## 8. Electron Spin and the Pauli Principle

The electron has a magnetic moment with two possible orientations.

$m_s$ the 4th quantum number for electron spin. Has two values: +1/2 and –1/2

Because 2 electrons in the same atom can have the same n, $\ell$, and $m_\ell$, :

Pauli Exclusion Principle: No two electrons in an atom can have the same four quantum numbers, therefore because an orbital can only hold two electrons they must have opposite spins.

## 9. Polyelectronic Atoms

**Electron Correlation Problem**: In atoms with more than one electron difficulties arise because one can not know the pathways nor repulsions among the electrons.
The electron is singled out in such a manner that the nuclear attraction and the average repulsion of all of the other electrons is treated as one.

The more effectively an orbital allows its electrons to penetrate (toward the nucleus) the shielding electrons (those electrons between the electron under study and the nucleus) the lower the energy of that orbital. $s < p < d$

## 10. The History of the Periodic Table

The quantum mechanical model explains the periodicity of chemical properties.

## 11. The Aufbau Principle and the Periodic Table

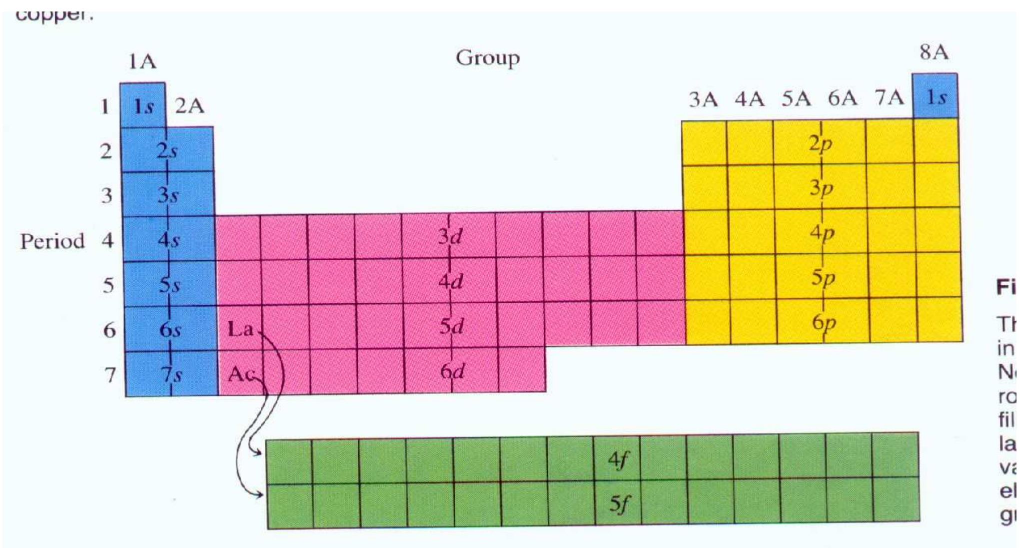
**Aufbau Principle** of building up atoms by adding electrons.
**Hund's Rule**: The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli Principle in a particular set of degenerate orbitals. For example: The 2p sublevel (-1, 0, +1) has three degenerate orbitals $\_\_{x}$ $\_\_{y}$ $\_\_{z}$. Electrons are added in a fashion so that the electrons "spread-out" and occupy their own orbitals before pairing up with opposite spins.

Oxygen' 6$^{th}$ ($1s^2 2s^2 sp^4$) electron will occupy an orbital with opposite spin.

**Valence Electrons**: electrons occupying the outermost principal quantum level of an atom. These electrons are involved in bonding. Elements within the same vertical group (family) of the periodic table have the same number of valence electrons. Indicated by the roman numeral headings. Ex. IIIA has 3 valence electrons. These Main Groups are called the Representative elements.
**Core Electrons**: inner electrons, not the valence electrons.
**Noble Gas Shorthand Notation**: Using the preceding Noble Gas in the electron configuration.

Ex. ${}_{15}P = 1s^2 2s^2 2p^6 3s^2 3p^3$ or $[Ne]3s^2 3p^3$

**Periodic Block Filling**: s, p, d, and f



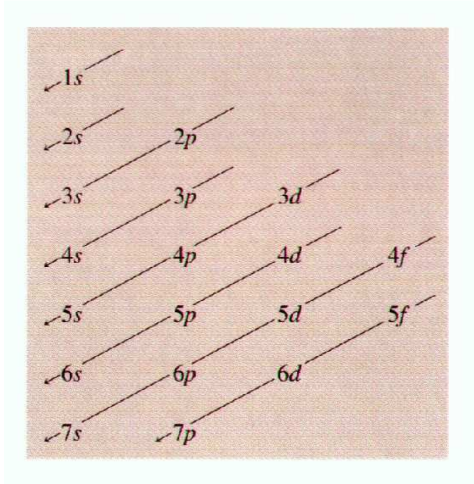

**The Cr and Cu exception**: (disagreement on the reason, except to say that the orbitals are half filled.

Cr = $[Ar]4s^1 3d^5$ Expected is $[Ar]4s^2 3d^4$

Cu = $[Ar]\ 4s^1 3d^{10}$ Expected is $[Ar]4s^2 3d^9$

IUPAC has established a new table that has the family columns numbered 1-18. This number indicates the number of *s*, *p*, and *d* electrons that have been added since the last noble gas.

**Aufbau summary diagram**:




**Homework for Study: P.321 #20, 21, 26, 28, 58, 59, 60, 62, 63, 64, 65, 66, 73, 74, 75, 76, 79, 80, 82, 124, 130, 131**