ENTRI

QUANTUM NUMBERS, ATOMIC ORBITALS, AND ELECTRON CONFIGURATIONS

Quantum Numbers and Atomic Orbitals

By solving the Schrödinger equation ($H\psi = E\psi$), we obtain a set of mathematical equations, called **wave functions** (ψ), which describe the probability of finding electrons at certain energy levels within an atom.

A wave function for an electron in an atom is called an **atomic orbital**; this atomic orbital describes a region of space in which there is a high probability of finding the electron. Energy changes within an atom are the result of an electron changing from a wave pattern with one energy to a wave pattern with a different energy (usually accompanied by the absorption or emission of a photon of light).

Each electron in an atom is described by four different **quantum numbers**. The first three (n, l, m_l) specify the particular orbital of interest, and the fourth (m_s) specifies how many electrons can occupy that orbital.

1. **Principal Quantum Number (n): $n = 1, 2, 3, \ldots, 8$.**

Specifies the **energy** of an electron and the **size** of the orbital (the distance from the nucleus of the peak in a radial probability distribution plot). All orbitals that have the same value of n are said to be in the same **shell** (**level**). For a hydrogen atom with n=1, the electron is in its *ground state*; if the electron is in the n=2 orbital, it is in an *excited state*. The total number of orbitals for a given n value is n^2.

2. **Angular Momentum (Secondary, Azimunthal) Quantum Number (l): $l = 0, \ldots, n-1$.**

Specifies the **shape** of an orbital with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of orbitals called **subshells** (**sublevels**). Usually, a letter code is used to identify l to avoid confusion with n:

	l	0	1	2	3	4	5	. . .
Letter	*s*	*p*	*d*	*f*	*g*	*h*	. . .	

The subshell with n=2 and l=1 is the 2*p* subshell; if n=3 and l=0, it is the 3*s* subshell, and so on. The value of l also has a slight effect on the energy of the subshell; the energy of the subshell increases with l (s < p < d < f).

3. **Magnetic Quantum Number (m_l): $m_l = -l, \ldots, 0, \ldots, +l$.**

Specifies the **orientation in space** of an orbital of a given energy (*n*) and shape (*l*). This number divides the subshell into individual **orbitals** which hold the electrons; there are 2*l*+1 orbitals in each subshell. Thus the *s* subshell has only one orbital, the *p* subshell has three orbitals, and so on.

4. Spin Quantum Number (m_s): m_s = +½ or -½.

Specifies the **orientation of the spin axis** of an electron. An electron can spin in only one of two directions (sometimes called *up* and *down*).

The **Pauli exclusion principle** (Wolfgang Pauli, Nobel Prize 1945) states that *no two electrons in the same atom can have identical values for all four of their quantum numbers*. What this means is that no more than **two** electrons can occupy the same orbital, and that two electrons in the same orbital must have **opposite spins**.

Because an electron spins, it creates a magnetic field, which can be oriented in one of two directions. For two electrons in the same orbital, the spins must be opposite to each other; the spins are said to be **paired**. These substances are not attracted to magnets and are said to be **diamagnetic**. Atoms with more electrons that spin in one direction than another contain **unpaired** electrons. These substances *are* weakly attracted to magnets and are said to be **paramagnetic**.

Table of Allowed Quantum Numbers

						Number of	Orbital	Number of
			n	*l*	m_l	orbitals	Name	electrons
1	0	0	1	1*s*	2			
2	0	0	1	2*s*	2			
				1	-1, 0, +1	3	2*p*	6
3	___	_____	___	___	___			
				___	_____	___	___	___
				___	_____	___	___	___
4	___	_____	___	___	___			
				___	_____	___	___	___
				___	_____	___	___	___
				___	_____	___	___	___
5	___	_____	___	___	___			
				___	_____	___	___	___
				___	_____	___	___	___

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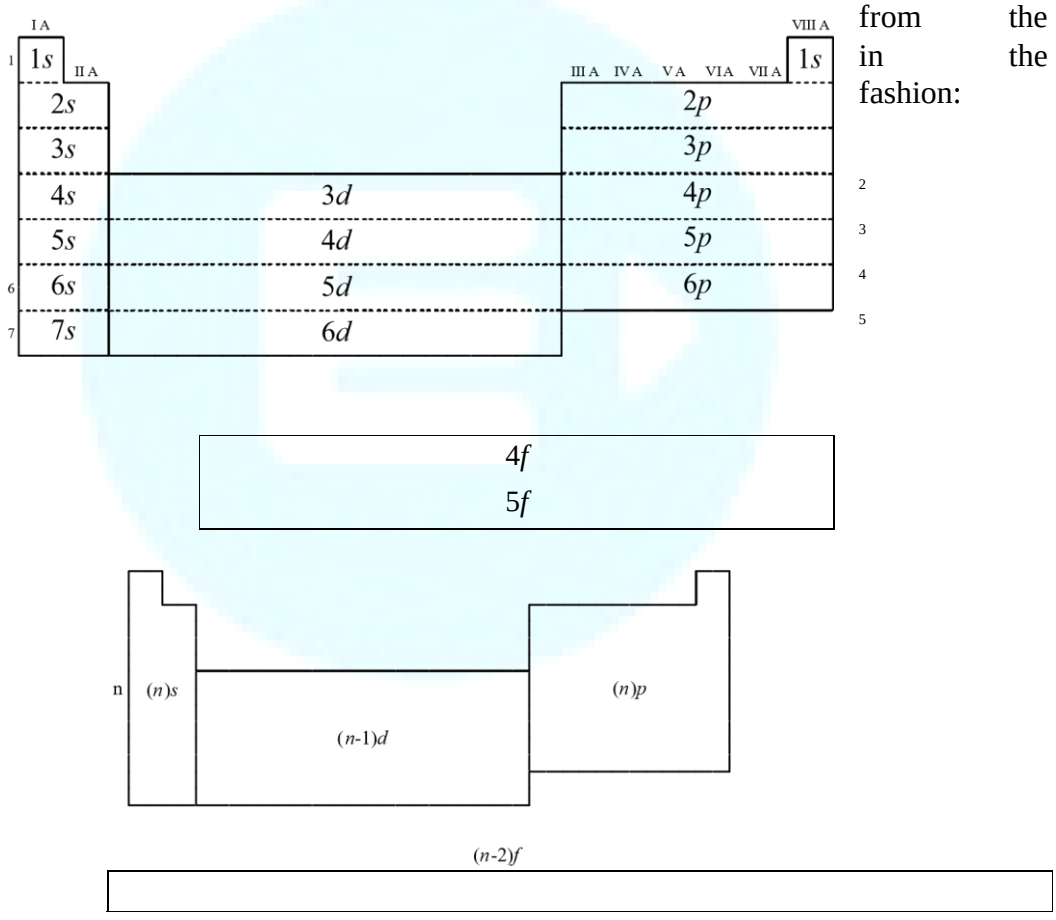
Writing Electron Configurations

The distribution of electrons among the orbitals of an atom is called the **electron configuration**. The electrons are filled in according to a scheme known as the **Aufbau principle** ("building-up"), which corresponds (for the most part) to increasing energy of the subshells:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f

It is not necessary to memorize this listing, because the order in which the electrons are filled in can be read from the periodic table in the following fashion:



In electron configurations, write in the orbitals that are occupied by electrons, followed by a superscript to indicate how many electrons are in the set of orbitals (e.g., H $1s^1$)

Another way to indicate the placement of electrons is an **orbital diagram**, in which each orbital is represented by a square (or circle), and the electrons as arrows pointing up or down (indicating the

electron spin). When electrons are placed in a set of orbitals of equal energy, they are spread out as much as possible to give as few paired electrons as possible (**Hund's rule**).

In a **ground state** configuration, all of the electrons are in as low an energy level as it is possible for them to be. When an electron absorbs energy, it occupies a higher energy orbital, and is said to be in an **excited state**.

Properties of Monatomic Ions

The electrons in the *outermost shell* (the ones with the highest value of *n*) are the most energetic, and are the ones which are exposed to other atoms. This shell is known as the **valence shell**. The inner, *core* electrons (*inner shell*) do not usually play a role in chemical bonding.

Elements with similar properties generally have similar outer shell configurations. For instance, we already know that the alkali metals (Group I) always form ions with a +1 charge; the "extra" s^1 electron is the one that's lost:

IA	Li	$1s^2 2s^1$	Li^+	$1s^2$
IA	Na	$1s^2 2s^2 2p^6 3s^1$	Na^+	$1s^2 2s^2 2p^6$
IA	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	K^+	$1s^2 2s^2 2p^6 3s^2 3p^6$

The next shell down is now the outermost shell, which is now full — meaning there is very little tendency to gain or lose more electrons. The ion's electron configuration is the same as the nearest noble gas — the ion is said to be **isoelectronic** with the nearest noble gas. Atoms "prefer" to have a filled outermost shell because this is more electronically stable.

- The Group IIA and IIIA metals also tend to lose all of their valence electrons to form cations.

IIA	Be	$1s^2 2s^2$	Be^{2+}	$1s^2$
IIA	Mg	$1s^2 2s^2 2p^6 3s^2$	Mg^{2+}	$1s^2 2s^2 2p^6$
IIIA	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	Al^{3+}	$1s^2 2s^2 2p^6$

- The Group IV and V metals can lose either the electrons from the *p* subshell, or from both the *s* and *p* subshells, thus attaining a **pseudo-noble gas configuration**.

IVA	Sn	[Kr] $4d^{10} 5s^2 5p^2$	Sn^{2+}	[Kr] $4d^{10} 5s^2$
			Sn^{4+}	[Kr] $4d^{10}$
IVA	Pb	[Xe] $4f^{14} 5d^{10} 6s^2 6p^2$	Pb^{2+}	[Xe] $4f^{14} 5d^{10} 6s^2$
			Pb^{4+}	[Xe] $4f^{14} 5d^{10}$
VA	Bi	[Xe] $4f^{14} 5d^{10} 6s^2 6p^3$	Bi^{3+}	[Xe] $4f^{14} 5d^{10} 6s^2$
			Bi^{5+}	[Xe] $4f^{14} 5d^{10}$

- The Group IV - VII non-metals gain electrons until their valence shells are full (8 electrons).

IVA	C	$1s^2 2s^2 2p^2$	C^{4-}	$1s^2 2s^2 2p^6$

VA N $1s^2 2s^2 2p^3$ N^{3-} $1s^2 2s^2 2p^6$ VIA O $1s^2 2s^2 2p^4$ O^{2-} $1s^2 2s^2 2p^6$
VIIA F $1s^2 2s^2 2p^5$ F^- $1s^2 2s^2 2p^6$

- The Group VIII noble gases already possess a full outer shell, so they have no tendency to form ions.
  VIIIA Ne $1s^2 2s^2 2p^6$
  VIIIA Ar $1s^2 2s^2 2p^6 3s^2 3p^6$

- Transition metals (B-group) usually form +2 charges from losing the valence *s* electrons, but can also lose electrons from the highest *d* level to form other charges.
  B-group Fe $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$ Fe^{2+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$
  Fe^{3+} $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$