Chemistry 151: Basic Chemistry

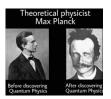


Electrons in Atoms

From previous sections, we know that protons and neutrons are in the nucleus... but what about the electrons?

Most of chemical reactions involve transferring electrons from reactant(s) to product(s), so knowledge of their location is critical.

Quantum physics delivers us answers... but they might make you think twice about the nature of our reality!



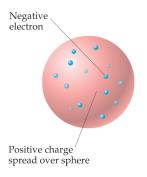
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The Plum Pudding Model of the Atom

JJ Thomson (discoverer of the electron) proposed the "plum pudding" model for the atom (and electrons) in 1904.

Large volume, negative "spheres" in a positive "cloud" of low density

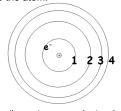
Rutherford's Gold Foil
Experiment proposed the
correct (current) model for the
nucleus
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The Bohr Model of the Atom

Niels Bohr proposed electrons exist in "orbits" - shells - around an atom

Electrons want to have the lowest energy possible, thus will occupy orbits closest to the nucleus (the ground state) – unless energy is added to the atom.



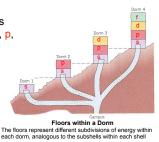
Ground state (lowest energy electronic configuration) for the Hydrogen atom.

Limitations of the Bohr Model

Bohr model worked great for H, not so great for other atoms

Schrödinger and others built a better model: **quantum mechanics**, where energy levels are split into *subshells* labeled s, p, d, and f.

The maximum number of sublevels per energy level = energy level number



Electronic Structure of Atoms

Quantum mechanical model of atomic structure gives info on electrons

Electrons restricted to moving within a certain region of space in atom - not free to "move about".

Position depends on the amount of energy the electron has.



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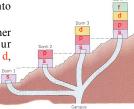
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Electronic Structure of Atoms

Energies of electrons are quantized, or restricted to having only certain values.

This means that electrons in an atom are grouped around the nucleus into shells.

Within the shells, electrons are further grouped into subshells of four different types, identified as s, p, d, and f, in order of increasing energy



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The floors represent different subdivisions of energy within each dorm, analogous to the subshells within each shell

Shell number: 1 2 3 4

Subshell designation: s s , p s , p , d s , p , d , f

From quantum mechanics we find:

- The first shell has only a s subshell
- The second shell has a s and p subshell
- The third shell has a s, p and d subshell.
- The fourth shell has a s, p, d, and f subshell.

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The number of subshells is equal to the shell number (ex: shell number 3 has 3 subshells)

Within each subshell, electrons are further grouped into orbitals, regions of space within an atom where the electrons are likely to be found. Each orbital holds two electrons.

There are different numbers of orbitals within the various subshells:

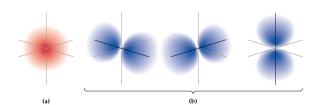
Shell number:	1	2	3	4
		$\overline{}$	$\overline{}$	$\overline{}$
Subshell designation:	s	s , p	s, p, d	s , p , d , f
Number of orbitals:	1	1 3	1 3 5	1 3 5 7

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Shapes of Orbitals

Orbitals have different shapes:

- Orbitals in s subshells are spherical (a, below)
- Orbitals in *p* subshells are roughly dumbbell / infinity shaped (b, below)



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The overall electron distribution within an atom:

TABLE 3.2 Electron Distribution in Atoms							
Shell number:	1	2	3	4			
Subshell designation:	S	s, p	s, p, d	s, p, d, f			
Number of orbitals:	1	1 3	1 3 5	1 3 5 7			
Number of electrons:	2	2 6	2 6 10	2 6 10 14			
Total electron capacity:	2	8	18	32			

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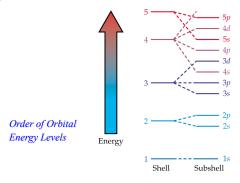
Electron Configurations

Electron Configuration: The exact arrangement of electrons in atom's shells and subshells. Rules to predict electron configurations:

- Electrons occupy the lowest-energy orbitals available, beginning with 1s and continuing in order shown on the next slide
- Each orbital holds only two electrons which must have opposite spin ("up" and "down")
- If two or more orbitals with the same energy: each orbital gets one electron before any orbital gets two.

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Notice *order* of electron filling... *important!* Each orbital holds *only* two electrons



Electron Configurations - Overview



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Ground State Electron Configurations

Fill electrons into the lowest energy sublevels first.

 $\label{eq:Relative energy of sublevels:} Relative energy of sublevels: \\ 1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s$

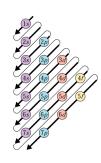
Procedure:

Start with a bare nucleus and fill electrons into the lowest energy sublevel first (1s), then moving on when each sublevel reaches its maximum number of electrons. Stop when you run out of electrons.

Each s subshell holds 2 electrons; each p subshell holds 6, d holds 10, f holds 14, etc.

This means that 1s, 2s, 3s, 4s, etc. - each of them holds only 2 electrons! Likewise 2p, 3p, 4p, etc. holds 6 electrons, etc.

The Aufbau Diagram



Aufbau diagram shows electron filling order (start at 1s and move down by arrow)

Each *s* orbital holds 2 electrons Each *p* orbital holds 6 electrons Each *d* orbital holds 10 electrons Each *f* orbital holds 14 electrons

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Electronic configuration of Magnesium:

Magnesium (Z=12) has 12 protons and 12 electrons

8 electrons in second shell
2 electrons in first shell

Mg (atomic number 12): $1s^2 2s^2 2p^6 3s^2$

Electronic configuration of Boron:

Boron (Z=5) has 5 protons and 5 electrons

B
$$1s^2 2s^2 2p^1$$
 or $\frac{\uparrow\downarrow}{1s^2} \frac{\uparrow\downarrow}{2s^2} \underbrace{\uparrow}_{2p^1}$

Orbital Box Notation

Boron shown with "spectroscopic" ($1s^2 2s^2 2p^1$) and orbital box notation (on the right)

Orbital box shows if atoms are paramagnetic (odd electron by itself) or diamagnetic (every up electron has a down electron.)

When filling in electrons, use 1 electron per box in a subshell, only pair when no more empty orbitals

B
$$1s^2 2s^2 2p^1$$
 or $\frac{\uparrow \downarrow}{1s^2} \frac{\uparrow \downarrow}{2s^2} \frac{\uparrow}{2s^2}$

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Boron is paramagnetic (up electron without down)

Orbital Box Notation

Boron is paramagnetic (one unpaired single electron in 2p subshell)

B
$$1s^2 2s^2 2p^1$$
 or $\frac{\uparrow \downarrow}{1s^2} \frac{\uparrow \downarrow}{2s^2} \frac{\uparrow}{2s^2}$

Magnesium is diamagnetic (every "up" electron has a "down" electron, no unpaired electrons)

$$\mathbf{Mg} \qquad \frac{\uparrow\downarrow}{1s^2} \quad \frac{\uparrow\downarrow}{2s^2} \quad \underbrace{\frac{\uparrow\downarrow}{2p^6}}_{2p^6} \quad \frac{\uparrow\downarrow}{3s^2}$$

Paramagnetic species affected by magnetic fields, more reactive **MAR**

paramagnetic C $1s^2 2s^2 2p^2$ or $\frac{\uparrow\downarrow}{1s^2} \frac{\uparrow\downarrow}{2s^2} \frac{\uparrow}{2s^2}$

Electron Configurations and the Periodic Table

The periodic table can be divided into four regions or blocks of elements according to the shells and subshells as shown on next slide:



H: 1s1 He: 1s²

Configurations These are "s-block" elements Li: 1s22s1

Test Yourself: Electron

Be: 1s22s2

B:

C: N:

O:

F:

Ne:

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For Sodium:

Group 1A

Atomic number = 11

1s2 2s2 2p6 3s1 or

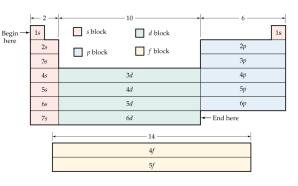
"neon core" + 3s1

[Ne] 3s1 (uses noble gas notation)

All Group 1A elements have [core] ns1 configurations:

- K: [Ar] 4s¹
- Rb: [Kr] 5s1
- Cs: [Xe] 6s¹





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Electron configurations and the periodic table

Valence Shell and Electrons

Valence Shell: Outermost shell of an atom.

Valence electrons: Electrons in the outermost shell of an atom. These electrons are loosely held and are most important in determining an element's properties and reactivities. Example:

$$\mathbf{P} \qquad \frac{\uparrow\downarrow}{1s^2} \quad \frac{\uparrow\downarrow}{2s^2} \qquad \underbrace{\uparrow\downarrow}_{2p^6} \stackrel{\uparrow\downarrow}{\longrightarrow} \qquad \frac{\uparrow\downarrow}{3s^2} \qquad \underbrace{\uparrow}_{3p^3} \stackrel{\uparrow}{\longrightarrow}$$

P has five valence electrons $(3s^23p^3)$ in the 3rd valence shell

Valence Electrons

Valence electrons are those in the outermost energy level (the highest main energy level) in an atom. These are the most reactive elements in an atom!

Shortcut: the number of valence electrons = the group number

Ex: Carbon - Group IV - 4 valence electrons Ex: Bromine - Group VII - 7 valence electrons

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Test Yourself

What is the electron configuration for As? How many valence electrons in As?

What is the electron configuration for Ca? How many valence electrons in Ca?

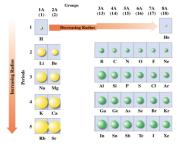
Periodic Properties: Atomic Size

Periodic Properties: properties of elements that repeat in a regular fashion as atomic number increases.

Atomic Size

Atomic size is described using the atomic radius; the distance from the nucleus to the valence electrons.

Size gets bigger as you go left and down the periodic table



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Atomic Radius Within A Group

Atomic radius increase: going down each group of representative elements.



Distance between the nucleus and a valence electron K atom

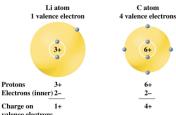
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Atomic Radius Across a Period

Going across a period left to right,

- an increase in number of protons increases attraction for valence electrons.
- · atomic radius decreases.

Protons



Ne atom 8 valence electrons

Test Yourself

Which neutral atom is larger: calcium or bromine?

Which neutral atom is larger: calcium or radium?

End of Chapter 3 Sections 3.3 - 3.5

