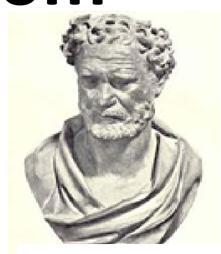
Unit 8: Atomic Theory

Quantum Mechanics

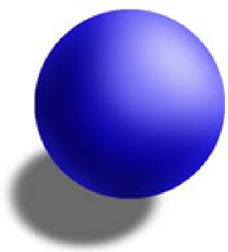
Unit 8: Atomic Theory

1. Historical Views of the Atom
2. The 'New' Look Atom
3. Electron Configurations
4. Electron Configurations & the Periodic Table
5. Quantum Numbers
6. Core Notation
7. Core Notation for Ions
8. Valence Electrons

1. Historical Views of the Atom

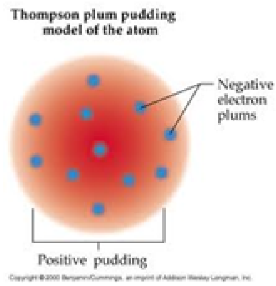


- Democritus & Leucippus (400 BC) - described atoms as invisible & indivisible

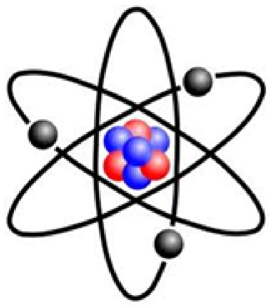


- Dalton(1808) - atoms like billiard balls (solid spheres)

- Thomson (1904) - “Plum Pudding” (Raisin Bun, Blueberry Muffin) - solid positive sphere with negative electrons imbedded in it



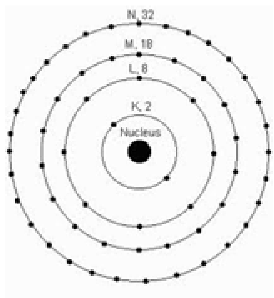
- Rutherford (1911) - positive charge concentrated in the nucleus with a cloud of negative electrons



http://regentsprep.org/Regents/physics/phys05/catomodel/ruther.htm

http://www.wwnorton.com/college/chemistry/gilbert2/tutorials/interface.asp?chapter=chapter_02&folder=rutherford_experiment

- Bohr (1913) - electrons can only be in certain orbits with certain amounts of energy (solar system model)



The old models of the atom have some practical uses:

- Protons and neutrons are in the nucleus
- Electrons are organized in orbitals around the nucleus
- The closer the orbital is to the nucleus, the lower the energy of the orbital

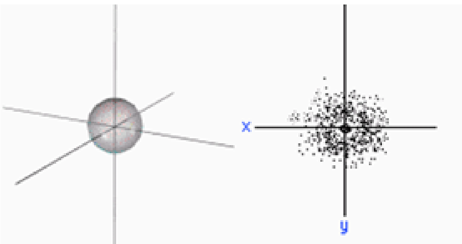
But…

- Electrons do not travel in specific pathways in the orbital as shown in the previous pictures
- Orbitals are not ‘trails’ around the nucleus

The Bohr model was replaced in the 1920s, just as quantum mechanics was beginning and your great-grandparents were very young or not even born!

2. The New Look Atom

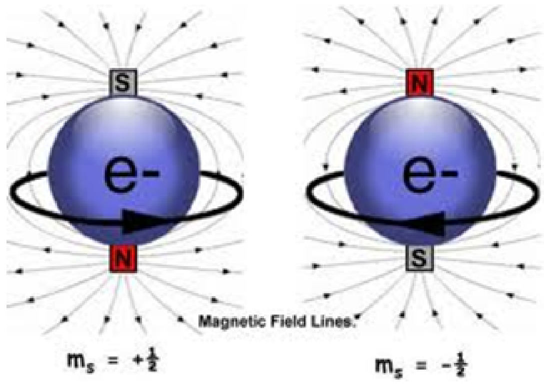
- Electrons are in orbitals, but orbitals are *clouds of probability* that show where an electron could be. The electron(s) are somewhere within the orbital, but we don't know where.



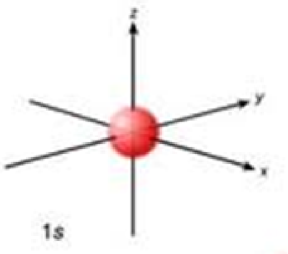
http://regentsprep.org/Regents/physics/phys05/catomodel/cloud.htm

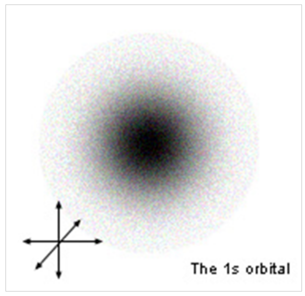
*For example, you may know your friend hangs out in the new wing at lunch time, but you don't know **exactly** where they will be at any time.*

- Orbitals have different sizes and shapes, depending on their energy level
- Every orbital can accommodate up to two electrons – each electron spins in a different direction



The Lowest Energy Orbital – 1s

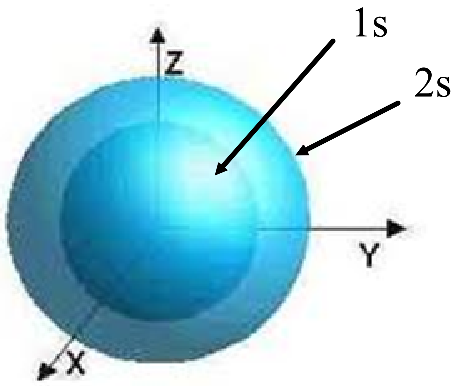




- Spherical in shape
- The smallest orbital
- Closest to the nucleus
- The lowest energy orbital in all atoms because it is closest to the nucleus
- Therefore, the electrons that occupy this orbital would be the lowest energy electrons because they have a higher probability of being closer to the nucleus than electrons in other, higher energy orbitals

2s Orbital

- The 1s orbital is the only one at energy level 1
- The next orbital is the 2s (energy level 2), which is the same as the 1s, only larger



Hydrogen

- How many electrons does hydrogen have?

1

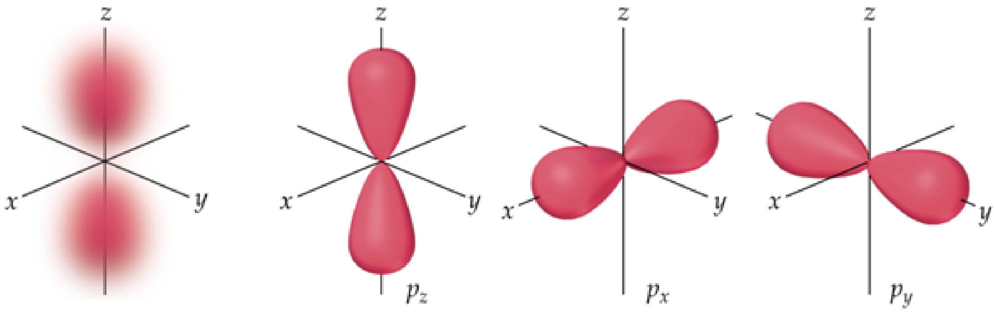
- In its stable state, the hydrogen electron is in the 1s (lowest energy) orbital. This is called the 'ground state' of hydrogen

If the electron becomes excited, it can be promoted to the 2s orbital (excited state), where it will eventually emit the excess energy and return to the 'ground state', the 1s level

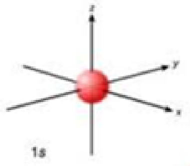
http://www.dlt.ncssm.edu/core/Chapter8-Atomic_Str_Part2/chapter8-Animations/ElectronOrbits.html

p orbitals

- The next orbitals after the 2s is the 3 different 2p orbitals. Each 2p orbital can hold up to two electrons, for a total of six electrons.
- The three 2p orbitals are the $2p_x$, $2p_y$, and $2p_z$ orbitals. http://www.dlt.ncssm.edu/core/Chapter8-Atomic_Str_Part2/chapter8-Animations/P-orbitalDiagram.html
- All three of these orbitals can be filled at once if there are enough electrons in the atom or ion.



Think back to Science 10…



- What was the electron shell pattern?

2, 8, 8, 18

Back to Chem 11. How many electrons can energy level 1 hold?

Level 1 has the 1s (1 orbital).

There are 2 electrons per orbital, so the first energy level will have 2 electrons.

How many electrons will energy level 2 hold?

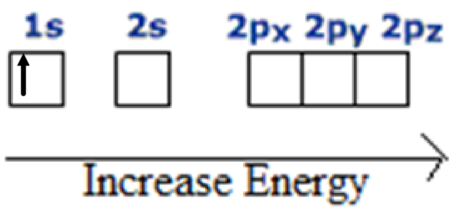
Level 2 will have these orbitals: 2s, 2px, 2py, 2pz

4 orbitals allows for 8 electrons

Notice a trend? – Our energy levels are the same as the 'shells' you learned about before

3. Electron Configurations

- Every atom or ion has an electron configuration - a map of where the electrons are relative to the nucleus.
- We represent the electrons in the *ground state* – the lowest energy arrangement



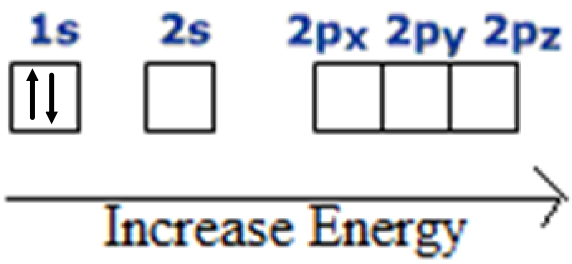
- Hydrogen only has one electron – what orbital would it be in? The 1s orbital (written as $1s^1$)

1 = energy level, s = orbital shape, 1 = # of electrons in the orbital

Where would helium's electrons be located?

- 2 electrons, so....
- We fill from the lowest energy orbital up, starting

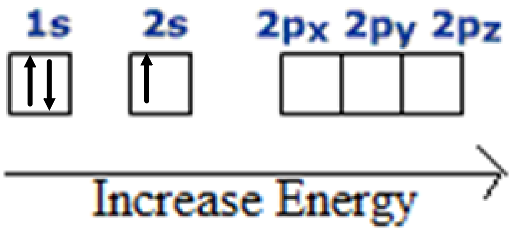
at 1s.



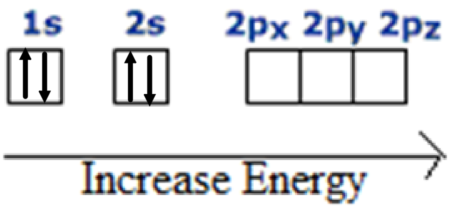
written notation: $1s^2$

Remember that in each orbital, the spin of each electron is opposite.

Lithium



Beryllium



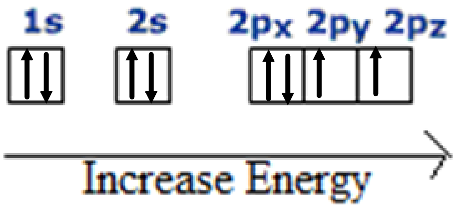
Hund's Rule

- p orbitals will fill by one electron going into each p orbital (p_x, p_y, p_z), and then doubling up after. This is a lower energy arrangement as it minimizes electron repulsion. This is called Hund's Rule.
- The same goes for d and f orbitals

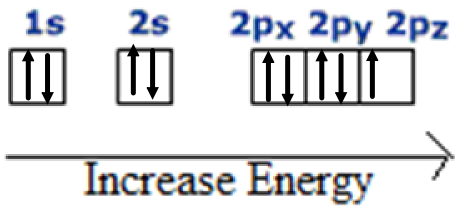
This is like sitting on a bus, you will sit in an empty row before sitting next to someone.

- Write electron configurations for oxygen, fluorine, and neon

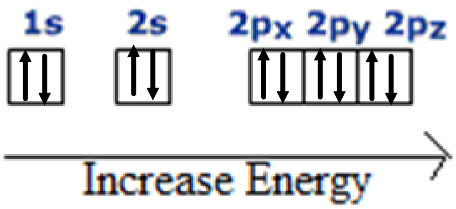
O:



F:



Ne:

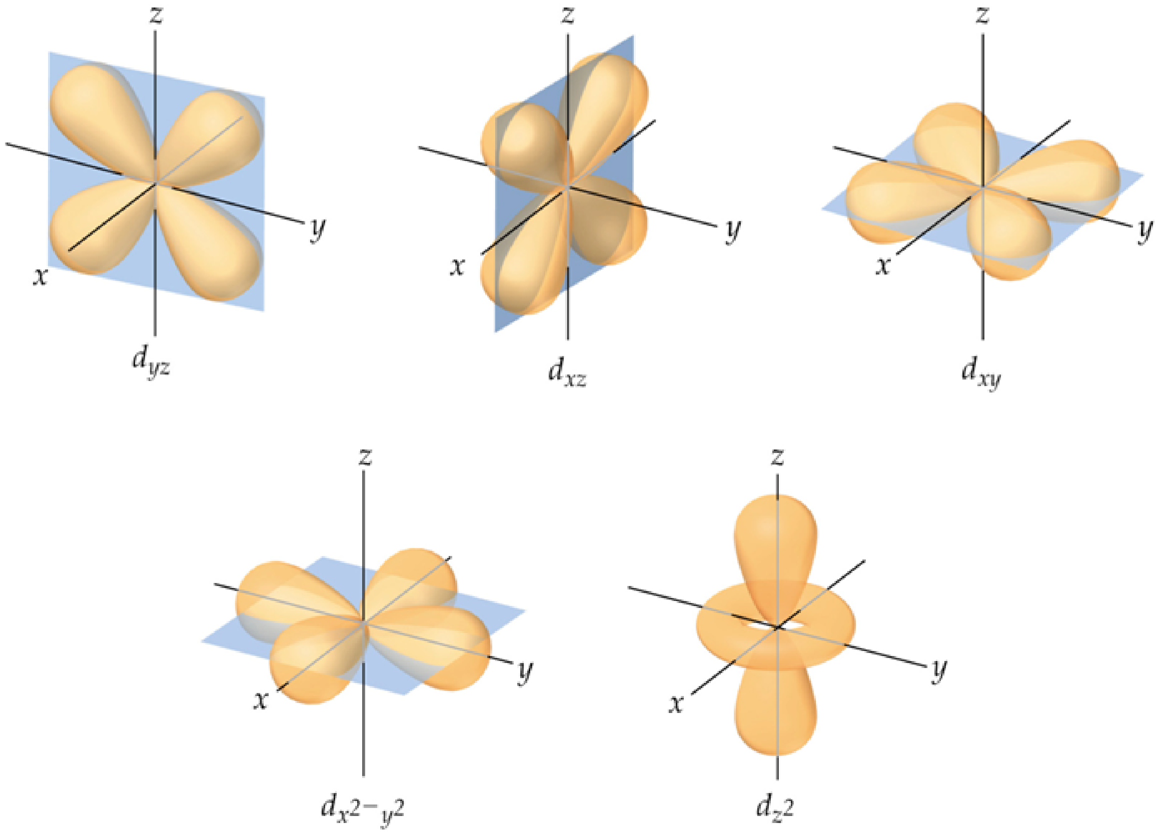


http://employees.oneonta.edu/viningwj/sims/atomic_electron_configurations_s1.html

Energy Level 3

- The third energy level has 3s, $3p_x$, $3p_y$, and $3p_z$ orbitals. They have the same shape as their energy level 2 counterparts, except they are larger and are higher energy.

- There are also five 3d orbitals that can each hold two electrons…

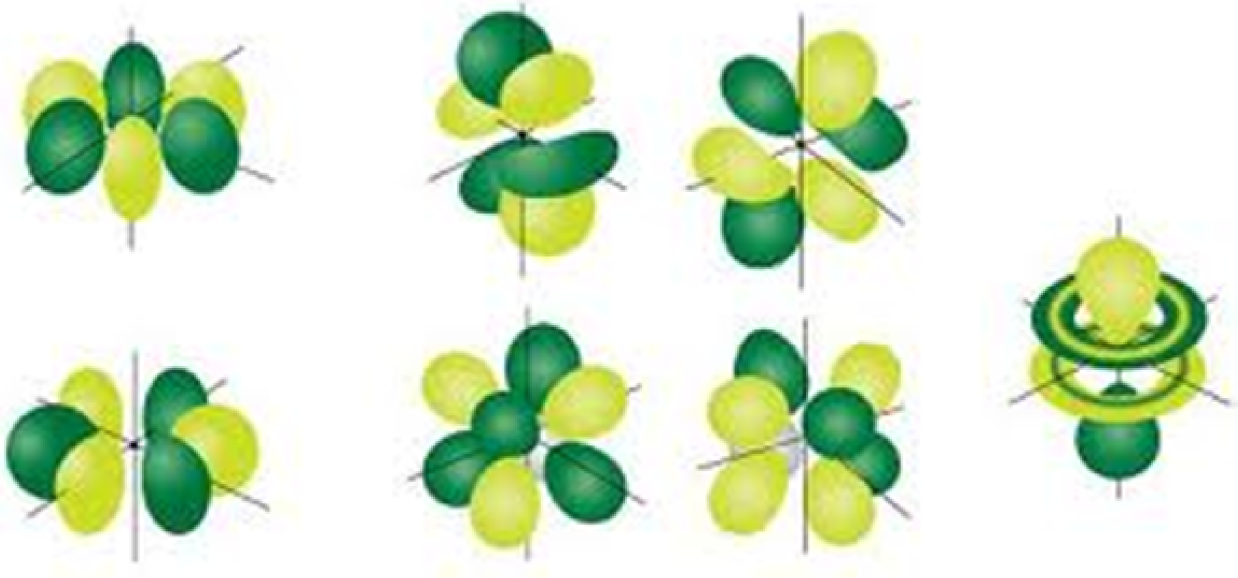

z
x
y
d_{yz}
z
x
y
d_{xz}
z
x
y
d_{xy}
z
x
y
$d_{x^2-y^2}$
z
x
y
d_{z^2}

Here's how 3s, the 3p, and the 3d look combined…

http://www.youtube.com/watch?v=K-jNgq16jEY

Energy Level 4

- The 4th energy level has a 4s orbital, three 4p orbitals, five 4d orbitals, and seven 4f orbitals. The s, p, and d orbitals look like the level 3 orbitals except they are larger and higher energy
- The seven 4f orbitals look like this…

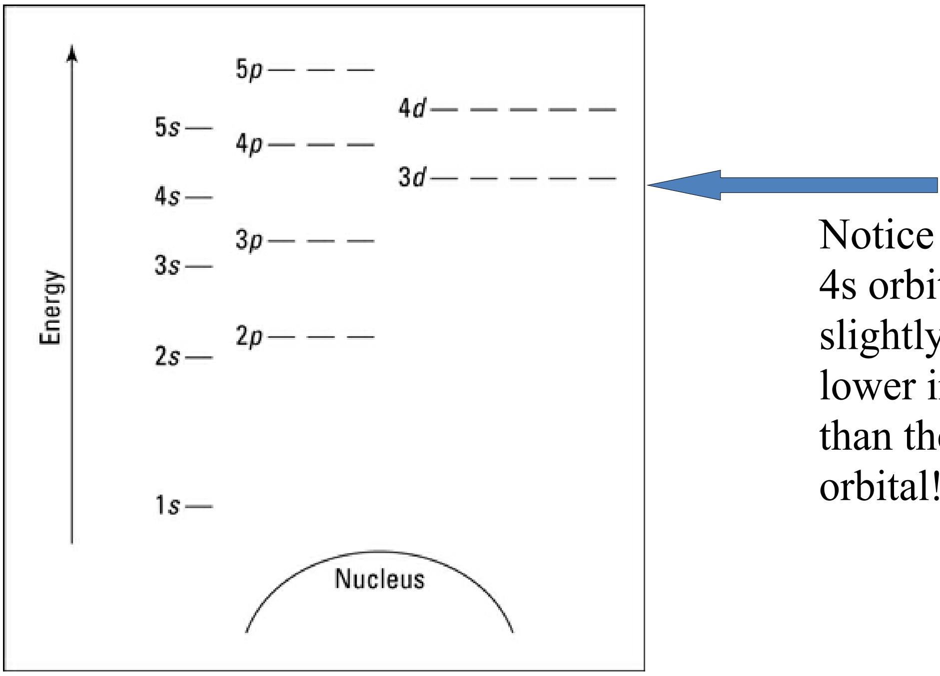


Energy Levels 5, 6, 7

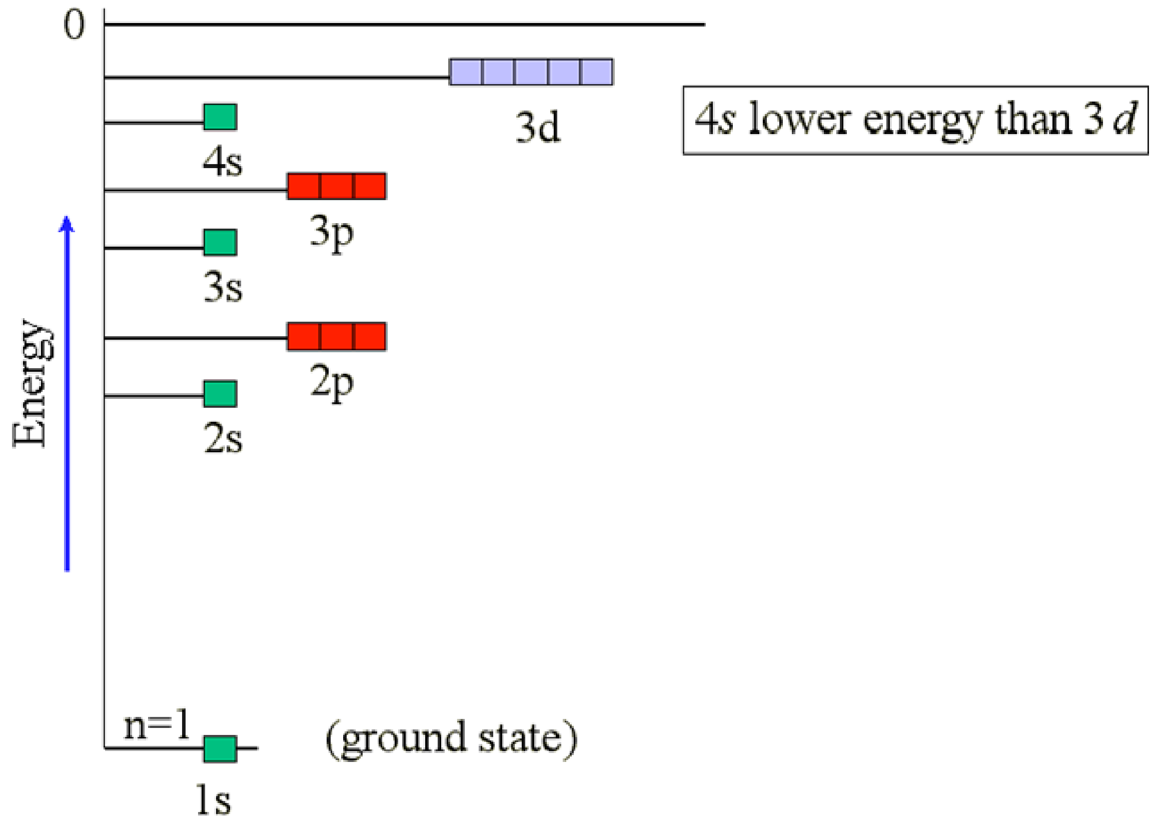
- Levels 5, 6, and 7 all have one s orbital, three p orbitals, five d orbitals, and seven f orbitals respectively
- As the energy level increases, both the size and energy of the orbitals increase

http://employees.oneonta.edu/viningwj/modules/CI_shapes_of_atomic_orbitals_7_14.html

- Orbitals will be filled from lowest to highest energy. See the relative energies of each orbital below:

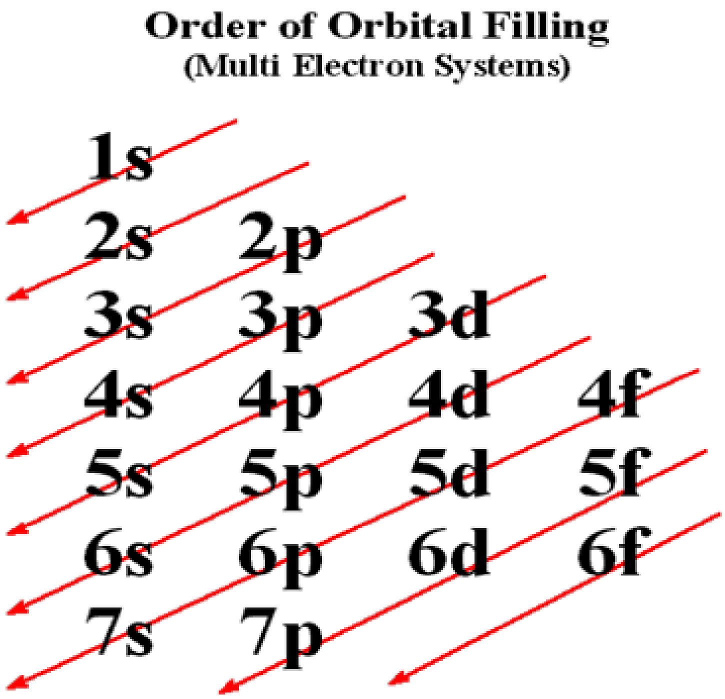


Notice that the 4s orbital is slightly lower in energy than the 3d orbital!



0
3d
4s lower energy than 3 d
4s
3p
3s
Energy
2p
2s
n=1
(ground state)
1s

Orbital Filling Order



Practice…

Give electron configurations for Silicon, Calcium, and Iron?

- Si : $1s^2 2s^2 2p^6 3s^2 3p^2$

- Ca : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

- Fe : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

http://www.learner.org/interactives/periodic/elementary_interactive.html

Answers

- Si $1s^2 2s^2 2p^6 3s^2 3p^2$
- Ca $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- Fe $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

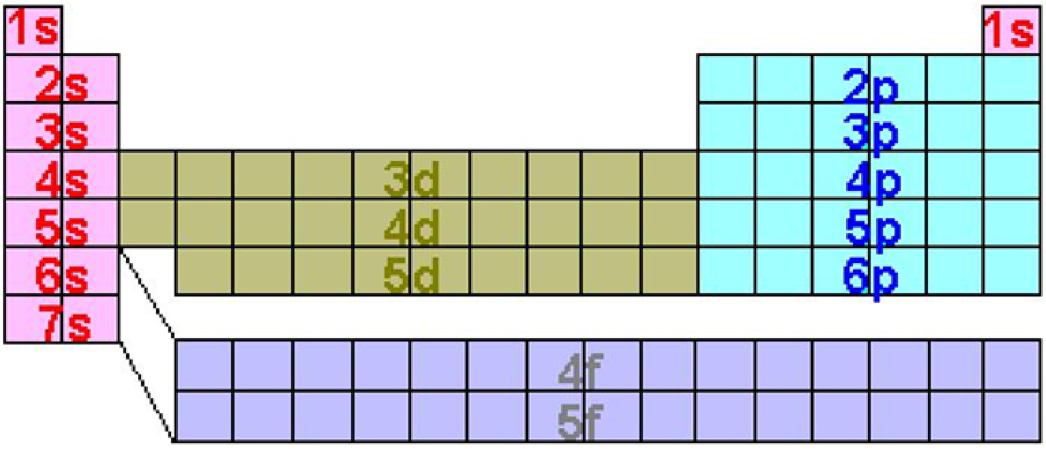
http://www.media.pearson.com.au/schools/cw/au_sch_lewis_cw2/int/electronConfig/0804.html

HOMEWORK:

Electron Configuration Worksheet

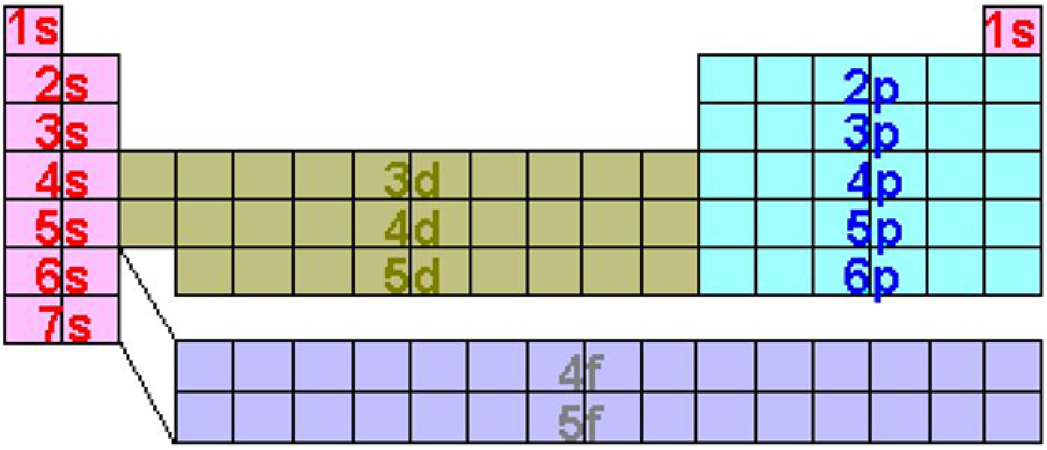
- Part I # 1 - 3
- Part 2 # 1-18

4. Electron Configurations and the Periodic Table



What order do the orbitals get filled again?

The periodic table gives the order by its layout!
1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d



Trends

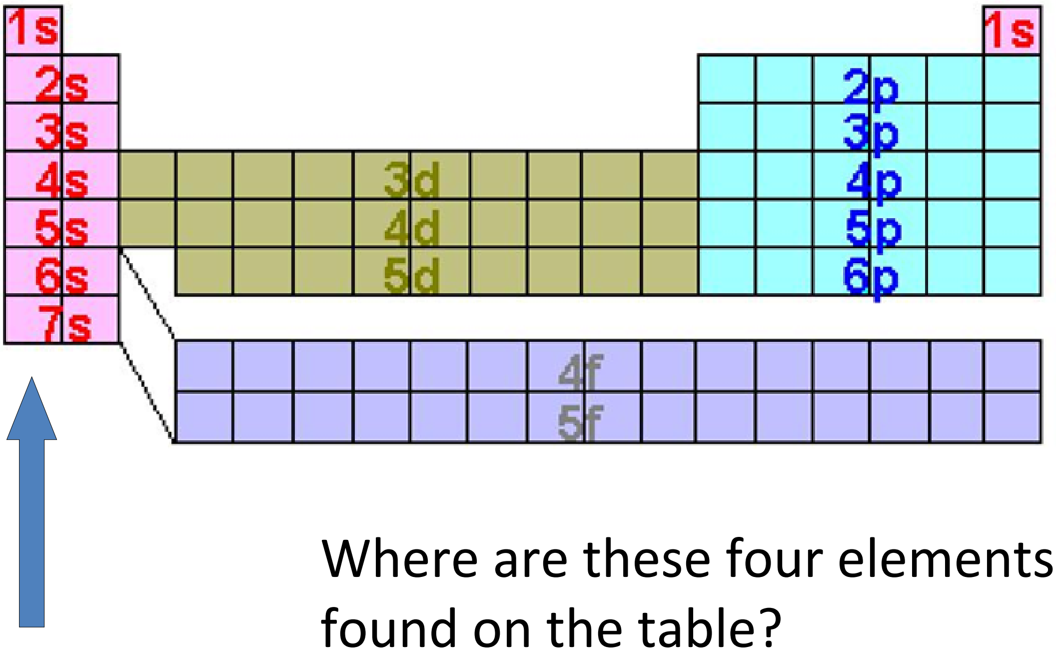
- ***Periodic Table Trends*** – The periodic table shows which order to fill orbitals.
- Give the electron configurations for hydrogen, lithium, sodium, and potassium.

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

K: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

- What is similar about each config?

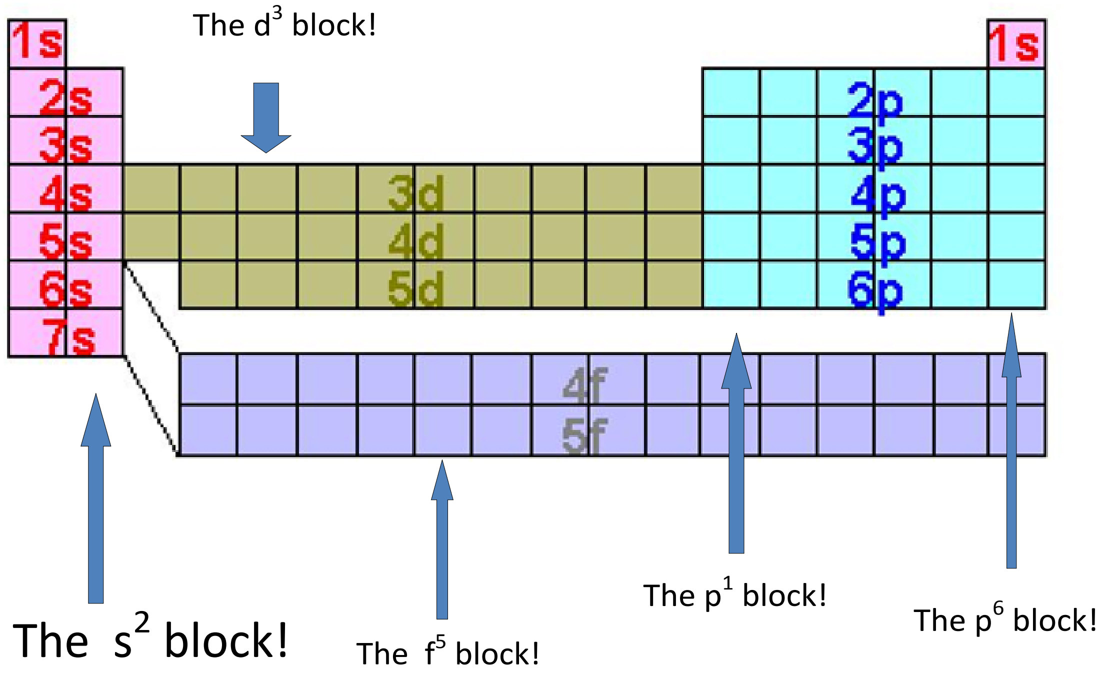
They all end in s^1



Where are these four elements found on the table?

In the first column -

The s^1 block! - which is why they are in the same family and have similar chemical properties (the alkali family)!


The d3 block!
1s
2s
3s
4s
5s
6s
7s
3d
4d
5d
1s
2p
3p
4p
5p
6p
4f
5f
The s2 block!
The f5 block!
The p1 block!
The p6 block!

Fill up **4f orbitals** before **5d orbitals** and fill up **5f orbitals** before **6d orbitals.**

Adjustments to our periodic tables:

La is our first 4f orbital and Yb is our last 4f orbital. Therefore **Lu** is our first 5d orbital.

Ac is our first 5f orbital and No is our last 5f orbital. Therefore **Lr** is our first 6d orbital.

METALS ← | → NON-METALS

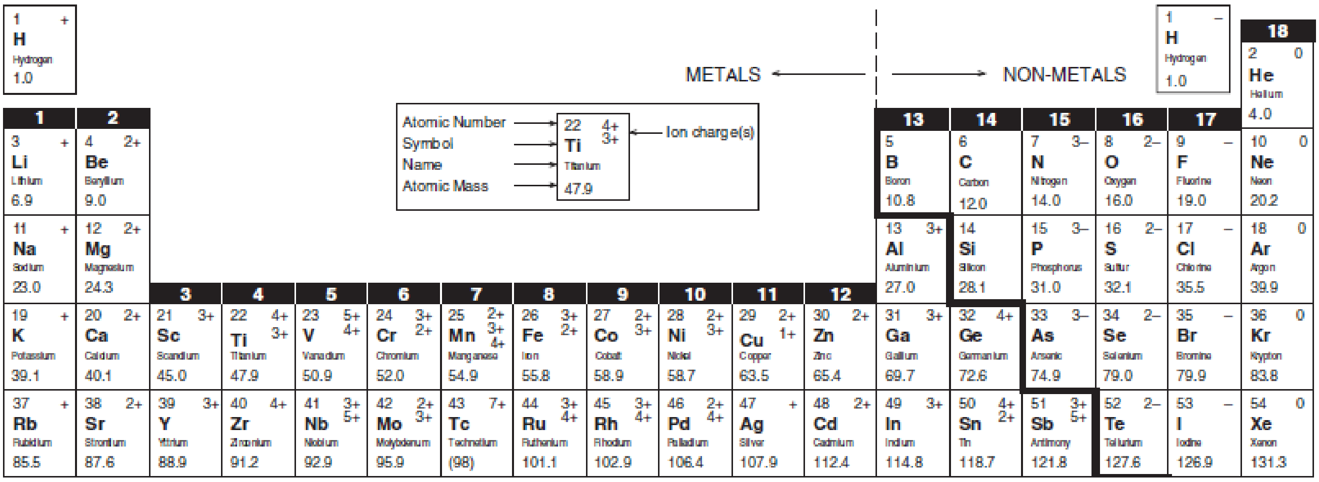
Atomic Number	Symbol	Name	Atomic Mass	Ion charge(s)
22	Ti	Titanium	47.9	4+ 3+

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 + **H** Hydrogen 1.0																1 − **H** Hydrogen 1.0	2 0 **He** Helium 4.0
3 + **Li** Lithium 6.9	4 2+ **Be** Beryllium 9.0											5 **B** Boron 10.8	6 **C** Carbon 12.0	7 3− **N** Nitrogen 14.0	8 2− **O** Oxygen 16.0	9 − **F** Fluorine 19.0	10 0 **Ne** Neon 20.2
11 + **Na** Sodium 23.0	12 2+ **Mg** Magnesium 24.3											13 3+ **Al** Aluminum 27.0	14 **Si** Silicon 28.1	15 3− **P** Phosphorus 31.0	16 2− **S** Sulfur 32.1	17 − **Cl** Chlorine 35.5	18 0 **Ar** Argon 39.9
19 + **K** Potassium 39.1	20 2+ **Ca** Calcium 40.1	21 3+ **Sc** Scandium 45.0	22 4+ 3+ **Ti** Titanium 47.9	23 5+ 4+ **V** Vanadium 50.9	24 3+ 2+ **Cr** Chromium 52.0	25 2+ 3+ 4+ **Mn** Manganese 54.9	26 3+ 2+ **Fe** Iron 55.8	27 2+ 3+ **Co** Cobalt 58.9	28 2+ 3+ **Ni** Nickel 58.7	29 2+ 1+ **Cu** Copper 63.5	30 2+ **Zn** Zinc 65.4	31 3+ **Ga** Gallium 69.7	32 4+ **Ge** Germanium 72.6	33 3− **As** Arsenic 74.9	34 2− **Se** Selenium 79.0	35 − **Br** Bromine 79.9	36 0 **Kr** Krypton 83.8
37 + **Rb** Rubidium 85.5	38 2+ **Sr** Strontium 87.6	39 3+ **Y** Yttrium 88.9	40 4+ **Zr** Zirconium 91.2	41 3+ 5+ **Nb** Niobium 92.9	42 2+ 3+ **Mo** Molybdenum 95.9	43 7+ **Tc** Technetium (98)	44 3+ 4+ **Ru** Ruthenium 101.1	45 3+ 4+ **Rh** Rhodium 102.9	46 2+ 4+ **Pd** Palladium 106.4	47 + **Ag** Silver 107.9	48 2+ **Cd** Cadmium 112.4	49 3+ **In** Indium 114.8	50 4+ 2+ **Sn** Tin 118.7	51 3+ 5+ **Sb** Antimony 121.8	52 2− **Te** Tellurium 127.6	53 − **I** Iodine 126.9	54 0 **Xe** Xenon 131.3
55 + **Cs** Cesium 132.9	56 2+ **Ba** Barium 137.3	57 3+ **La** Lanthanum 138.9	72 4+ **Hf** Hafnium 178.5	73 5+ **Ta** Tantalum 180.9	74 6+ **W** Tungsten 183.8	75 4+ 7+ **Re** Rhenium 186.2	76 3+ 4+ **Os** Osmium 190.2	77 3+ 4+ **Ir** Iridium 192.2	78 4+ 2+ **Pt** Platinum 195.1	79 3+ 1+ **Au** Gold 197.0	80 2+ 1+ **Hg** Mercury 200.6	81 1+ 3+ **Tl** Thallium 204.4	82 2+ 4+ **Pb** Lead 207.2	83 3+ 5+ **Bi** Bismuth 209.0	84 2+ 4+ **Po** Polonium (209)	85 − **At** Astatine (210)	86 0 **Rn** Radon (222)
87 + **Fr** Francium (223)	88 2+ **Ra** Radium (226)	89 3+ **Ac** Actinium (227)	104 **Rf** Rutherfordium (261)	105 **Db** Dubnium (262)	106 **Sg** Seaborgium (263)	107 **Bh** Bohrium (262)	108 **Hs** Hassium (265)	109 **Mt** Meitnerium (266)	110 **Ds** Darmstadtium (281)	111 **Rg** Roentgenium (272)	112 **Uub** Ununbium (285)	113 **Uut** Ununtrium (284)	114 **Uuq** Ununquadium (289)	115 **Uup** Ununpentium (288)	116 **Uuh** Ununhexium (292)	117 **Uus** Ununseptium (?)	118 **Uuo** Ununoctium (294)
Alkali Metals	Alkaline Earth Metals															Halogens	Noble Gases

58 3+ 4+ **Ce** Cerium 140.1	59 3+ 4+ **Pr** Praseodymium 140.9	60 3+ **Nd** Neodymium 144.2	61 3+ **Pm** Promethium (145)	62 3+ 4+ **Sm** Samarium 150.4	63 3+ 2+ **Eu** Europium 152.0	64 3+ **Gd** Gadolinium 157.3	65 3+ 4+ **Tb** Terbium 158.9	66 3+ **Dy** Dysprosium 162.5	67 3+ **Ho** Holmium 164.9	68 3+ **Er** Erbium 167.3	69 3+ 2+ **Tm** Thulium 168.9	70 3+ 2+ **Yb** Ytterbium 173.0	71 3+ **Lu** Lutetium 175.0
90 4+ **Th** Thorium 232.0	91 5+ 4+ **Pa** Protactinium 231.0	92 6+ 4+ 5+ **U** Uranium 238.0	93 5+ 3+ 4+ 6+ **Np** Neptunium (237)	94 4+ 6+ 3+ 5+ **Pu** Plutonium (244)	95 3+ 4+ 5+ 6+ **Am** Americium (243)	96 3+ **Cm** Curium (247)	97 3+ 4+ **Bk** Berkelium (247)	98 3+ **Cf** Californium (251)	99 3+ **Es** Einsteinium (252)	100 3+ **Fm** Fermium (257)	101 2+ 3+ **Md** Mendelevium (258)	102 2+ 3+ **No** Nobelium (259)	103 3+ **Lr** Lawrencium (262)

Based on mass of C-12 at 12.00.

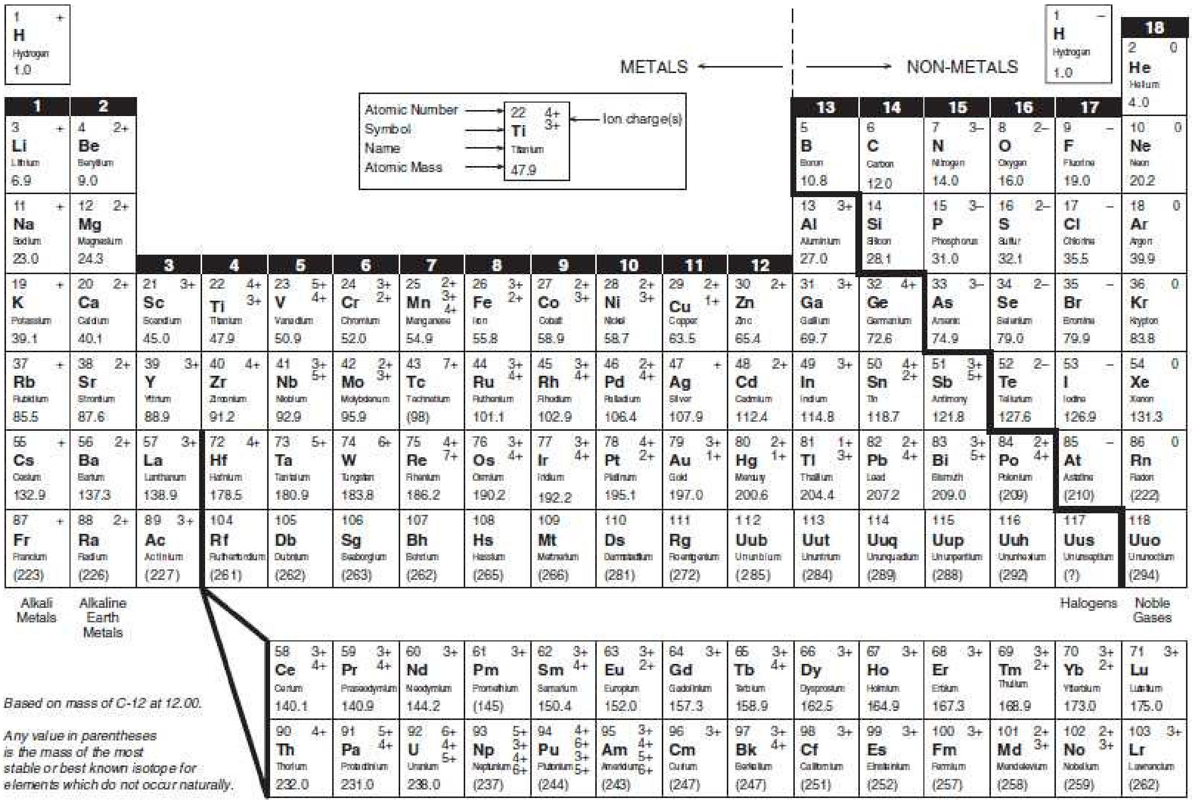
Any value in parentheses is the mass of the most stable or best known isotope for elements which do not occur naturally.



Give the electron configurations of:

Zn: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$

Se: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$



Pt: $1s^22s^22p^63s^23p^64s^23d^{10}4p^65s^24d^{10}5p^66s^24f^{14}5d^8$

5. Quantum Numbers

- Quantum numbers are a way of keeping track of all the different electrons in an atom or ion

- Each electron in an atom has a different set of 4 quantum numbers

Principal Quantum Number (n)

- tells what energy level the orbital occupies
- n values can be 1, 2, 3, 4, 5, 6, or 7

Show in electron configuration in red: $1s^2 2s^2$

- Energy and orbital size increases as the n value increases

Angular Quantum Number (L)

- L tells the shape of the orbital…
- is it an s, p, d, or f orbital?

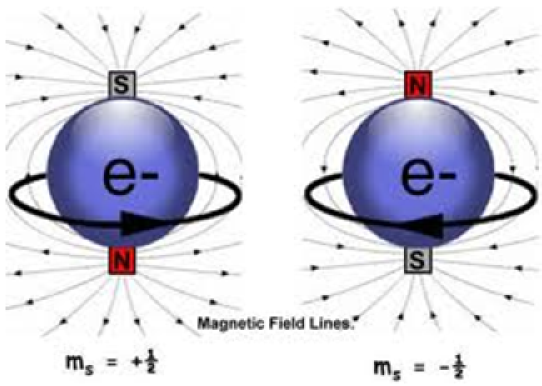
Magnetic Quantum Number (m_L)

- m tells the orientation of the orbital
- s has no orientation as it is a sphere
- p can be p_x, p_y, or p_z

- d and f are more complicated so you don't have to know these (5 for d and 7 for f)

Spin quantum number (m_s)

- m_s gives the spin of the electron…
- either +1/2 or –1/2



Pauli Exclusion Principle

Electrons can have one, two, or three of the same quantum numbers, but never all four. If all four quantum numbers are the same, we are describing the same electron!

Electrons in Oxygen:

n	L	m_L	m_s
1	s	-	+1/2
1	s	-	-1/2
2	s	-	+1/2
2	s	-	-1/2
2	p	x	+1/2
2	p	y	+1/2
2	p	z	+1/2
2	p	x	-1/2

6. Core Notation

- Give the electron configuration for Titanium

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$

- The ***core*** is the configuration that is identical to the <u>nearest *previous noble gas*</u> – then write the configuration for the remaining outer electrons

- Core Notation for Ti:

$[Ar]\ 4s^2 3d^2$

Practice…

- Give core notation for:

As: $[Ar]4s^2 3d^{10} 4p^3$

Cl: $[Ne]3s^2 3p^5$

In: $[Kr]5s^2 4d^{10} 5p^1$

Pm: $[Xe]6s^2 4f^5$

Bh: $[Rn]7s^2 5f^{14} 6d^5$

HOMEWORK:

Electron Configuration Worksheet

- Part III # 1 – 18 (Core Notation)
- Part IV # 1 – 8

7. Core Notation for Ions

Core Notation for Anions

- An anion is an ion with negative charge - meaning it has extra electrons
- The extra electrons go into the lowest energy available orbital

Give core notation for P^{3-}

Step 1: write core notation for atom

P: [Ne]$3s^2 3p^3$

Step 2: add on anionic charge to atom

P^{3-}: [Ne]$3s^2 3p^6$

Examples - Give Core Notation

I^-

I: $[Kr]5s^24d^{10}5p^5$

I^-: $[Kr]5s^24d^{10}5p^6$

As^{3-}

As: $[Ar]4s^23d^{10}4p^3$

As^{3-}: $[Ar]4s^23d^{10}4p^6$

Se^{2-}

Se: $[Ar]4s^23d^{10}4p^4$

Se^{2-}: $[Ar]4s^23d^{10}4p^6$

Core Notation for Cations

- positively charged ion
- Has less electrons than the neutral atom

RULE: Electrons are removed from p-orbitals first, then s-orbitals, then d-orbitals (<u>P</u>eople <u>S</u>hould <u>D</u>ream)

Give core notation for Ca^{2+}

Step 1: Write core notation for Ca atom

Ca: [Ar]$4s^2$

Step 2: Take off electrons according to P.S.D.

Ca^{2+}: [Ar]

Practice

- Give core notation for Fe^{2+}, Al^{3+}, Li^{+}, Mn^{2+}, Fe^{3+}, Pb^{4+}

Fe: $[Ar]4s^2 3d^6$

Fe^{2+}: $[Ar]3d^6$

Fe^{3+}: $[Ar]3d^5$

Al: $[Ne]3s^2 3p^1$

Al^{3+}: [Ne]

Li: $[He]2s^1$

Li^{+}: [He]

Mn: $[Ar]4s^2 3d^5$

Mn^{2+}: $[Ar]3d^5$

Pb: $[Xe]6s^2 4f^{14} 5d^{10} 6p^2$

Pb^{4+}: $[Xe]4f^{14} 5d^{10}$

Isoelectronic

- What do you notice about the electron configuration of many of the ions?

They have the same configuration as noble gases (and are happy)! Ions which have identical configurations to noble gases are said to be ***isoelectronic*** with the noble gas.

Atoms will strive to have the same stable configuration as noble gases, as noble gases have full p orbitals and exhibit extra stability

Core Notation for Ions Online

http://employees.oneonta.edu/viningwj/sims/atomic_electron_configurations_s2.html

http://www.media.pearson.com.au/schools/cw/au_sch_lewis_cw2/int/ionElectronConfigs/IonElectronConfigs.html

Stability of Full and Half-full *d* orbitals

- Any configuration that ends in ***d^4 or d^9*** will undergo electron elevation, meaning an *s* electron moves up to a *d* orbital to make it d^5 (half-full d) or d^{10} (full d)

Ag [Kr] $5s^2 4d^9$ is actually [Kr] $5s^1 4d^{10}$
Ag^+ [Kr] $5s^1 4d^9$ is actually [Kr] $4d^{10}$
Cr [Ar] $4s^2 3d^4$ is actually [Ar] $4s^1 3d^5$

The elevation of an s electron to a half- or fully-filled d orbital is due to the extra stability that results for the atom or ion
It is unexpected and a phenomenon that is not well explained! Chemists are still looking into this.

Find Core Notation for:

W: $[Xe]6s^2 4f^{14} 5d^4$ becomes $[Xe]6s^1 4f^{14} 5d^5$

Cu: $[Ar]4s^2 3d^9$ becomes $[Ar]4s^1 3d^{10}$

so **Cu⁺**: $[Ar]3d^{10}$

Summary of unit:
http://www.wwnorton.com/college/chemistry/gilbert2/tutorials/interface.asp?chapter=chapter_07&folder=orbital_filling

8. Valence Electrons for Atoms and Ions

Valence Electrons

- Valence electrons are the outer most electrons that take part in chemical reactions

- Valence electrons are all the electrons that are **not** in the core, and **not** in filled *d* or *f* orbitals

- Valence electrons can be used to bond with other atoms to make a compound

- Examples - Determine valence electrons for:

Al: [Ne]$3s^2 3p^1$ so 3 valence electrons

Ge: [Ar]$4s^2 3d^{10} 4p^2$ so 4 valence electrons

Cr: [Ar]$4s^2 3d^4$ becomes [Ar]$4s^1 3d^5$ so 6 valence

Xe: [Xe] so 0 valence electrons (it's a noble gas)

Ions

- Atoms become ions by gaining or losing valence electrons to achieve full orbitals

Examples - Determine valence electrons for:

Al^{3+}: [Ne] so 0 valence electrons (isoelectronic with Ne)

S^{2-}: [Ar] so 0 valence electrons (isoelectronic with Ar)

HOMEWORK:

- Electron Configuration Worksheet Parts 5-8

Unit Summary: http://kaffee.50webs.com/Science/activities/Chem/Activity.Electron.Configuration.html