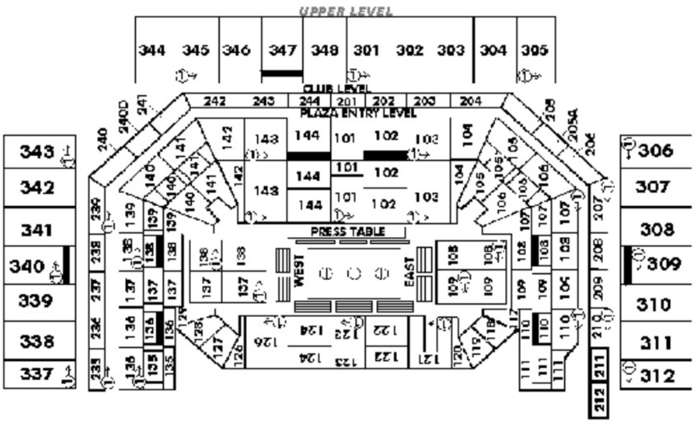
Quantum Mechanics

1. Using the Quantum Mechanical Model, we can determine the likelihood of finding an electron

2. The <u>Pauli Exclusion Principle</u> states that no two electrons in an atom can occupy the same orbital (they cannot have the same address)

3. There are four quantum numbers that can help us locate each electron in an atom. (find their address)



A. <u>Principle Quantum Number (n)</u>

a. The energy level of the electron

b. Determines the size of the orbital

c. Accepted values are n=1,2,3,4,5,6,7.

d. The higher the principle quantum number, the more energy the electron has.

1s 2s

B. Angular Momentum Quantum Number (ℓ)

a. Tells the energy sub-level

b. Tells you the shape of the orbital

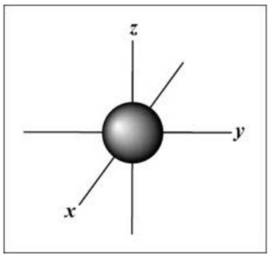
c. Depends upon the principal quantum number

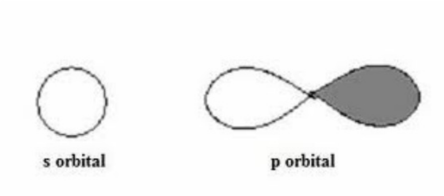
n-1 = ℓ --> *whatever you get, you also have the previous orbits (4-1 = 3,2,1, and 0)*

ℓ=0 s orbit
ℓ=1 p orbit
ℓ=2 d orbit
ℓ=3 f orbit

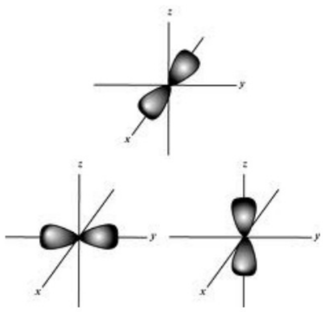
Example: n=3 ℓ=1
This refers to a 3p e^-

s-orbital

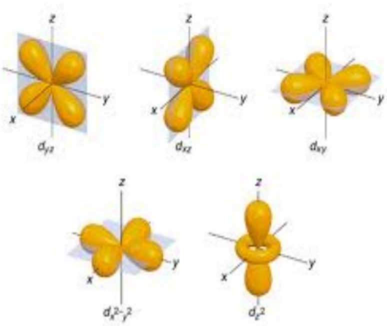


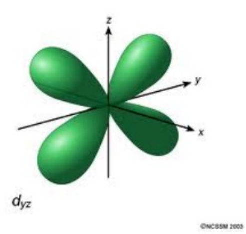


p-orbital

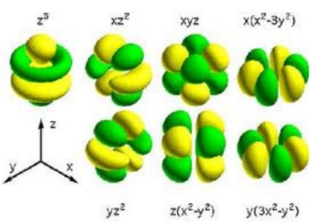


d-orbital





f-orbital



Maximum Capacities of Subshells and Principal Shells

n	1	2		3			4				...*n*
l	0	0	1	0	1	2	0	1	2	3	
Subshell designation	*s*	*s*	*p*	*s*	*p*	*d*	*s*	*p*	*d*	*f*	
Orbitals in subshell	1	1	3	1	3	5	1	3	5	7	
Subshell capacity	2	2	6	2	6	10	2	6	10	14	
Principal shell capacity	2	8		18			32				...$2n^2$

Hill, Petrucci, General Chemistry *An Integrated Approach* 1999, page 320

C. Magnetic Quantum Number (m_l)

a. Specifies the oreientation of a specific orbital

b. Tells you the exact orbital within each sublevel

c. Depends upon the angular momentum quantum number.

d. The pattern is: $m_l = -l\ ..., 0, ..., +l$

e. Thus, when $l = 0$, $m_l = 0$

when $l = 1$, $m_l = -1,0,+1$

when $l = 2$, $m_l = -2,-1,0,+1,+2$

when $l = 3$, $m_l = -3,-2,-1,0,+1,+2,+3$

The Periodic Table of the Elements

p-obitals

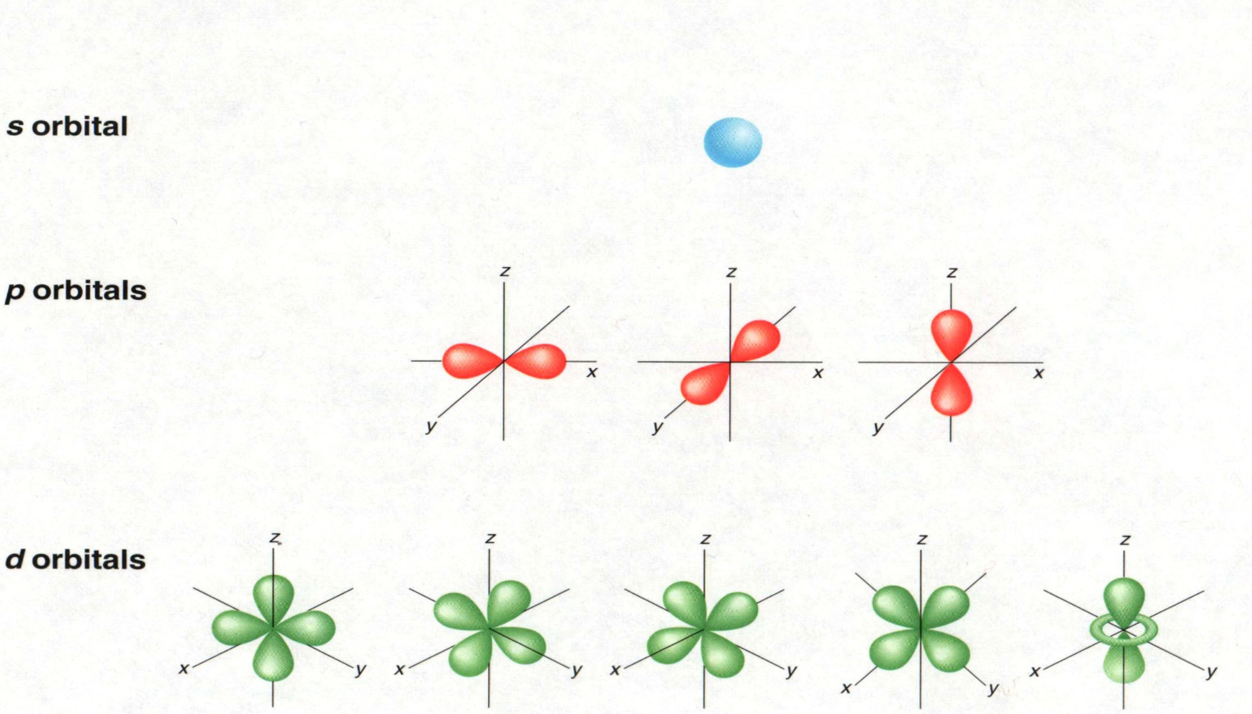
d-orbital

1 **H** Hydrogen 1.00794																	2 **He** Helium 4.003
3 **Li** Lithium 6.941	4 **Be** Beryllium 9.012182											5 **B** Boron 10.811	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.00674	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.9984032	10 **Ne** Neon 20.1797
11 **Na** Sodium 22.989770	12 **Mg** Magnesium 24.3050											13 **Al** Aluminum 26.981538	14 **Si** Silicon 28.0855	15 **P** Phosphorus 30.973761	16 **S** Sulfur 32.066	17 **Cl** Chlorine 35.4527	18 **Ar** Argon 39.948
19 **K** Potassium 39.0983	20 **Ca** Calcium 40.078	21 **Sc** Scandium 44.955910	22 **Ti** Titanium 47.867	23 **V** Vanadium 50.9415	24 **Cr** Chromium 51.9961	25 **Mn** Manganese 54.938049	26 **Fe** Iron 55.845	27 **Co** Cobalt 58.933200	28 **Ni** Nickel 58.6934	29 **Cu** Copper 63.546	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92160	34 **Se** Selenium 78.96	35 **Br** Bromine 79.904	36 **Kr** Krypton 83.80
37 **Rb** Rubidium 85.4678	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.90585	40 **Zr** Zirconium 91.224	41 **Nb** Niobium 92.90638	42 **Mo** Molybdenum 95.94	43 **Tc** Technetium (98)	44 **Ru** Ruthenium 101.07	45 **Rh** Rhodium 102.90550	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.8682	48 **Cd** Cadmium 112.411	49 **In** Indium 114.818	50 **Sn** Tin 118.710	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447	54 **Xe** Xenon 131.29
55 **Cs** Cesium 132.90545	56 **Ba** Barium 137.327	57 **La** Lanthanum 138.9055	72 **Hf** Hafnium 178.49	73 **Ta** Tantalum 180.9479	74 **W** Tungsten 183.84	75 **Re** Rhenium 186.207	76 **Os** Osmium 190.23	77 **Ir** Iridium 192.217	78 **Pt** Platinum 195.078	79 **Au** Gold 196.96655	80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98038	84 **Po** Polonium (209)	85 **At** Astatine (210)	86 **Rn** Radon (222)
87 **Fr** Francium (223)	88 **Ra** Radium (226)	89 **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 (269)	111 (272)	112 (277)	113	114				
				58 **Ce** Cerium 140.116	59 **Pr** Praseodymium 140.90765	60 **Nd** Neodymium 144.24	61 **Pm** Promethium (145)	62 **Sm** Samarium 150.36	63 **Eu** Europium 151.964	64 **Gd** Gadolinium 157.25	65 **Tb** Terbium 158.92534	66 **Dy** Dysprosium 162.50	67 **Ho** Holmium 164.93032	68 **Er** Erbium 167.26	69 **Tm** Thulium 168.93421	70 **Yb** Ytterbium 173.04	71 **Lu** Lutetium 174.967
				90 **Th** Thorium 232.0381	91 **Pa** Protactinium 231.03588	92 **U** Uranium 238.0289	93 **Np** Neptunium (237)	94 **Pu** Plutonium (244)	95 **Am** Americium (243)	96 **Cm** Curium (247)	97 **Bk** Berkelium (247)	98 **Cf** Californium (251)	99 **Es** Einsteinium (252)	100 **Fm** Fermium (257)	101 **Md** Mendelevium (258)	102 **No** Nobelium (259)	103 **Lr** Lawrencium (262)

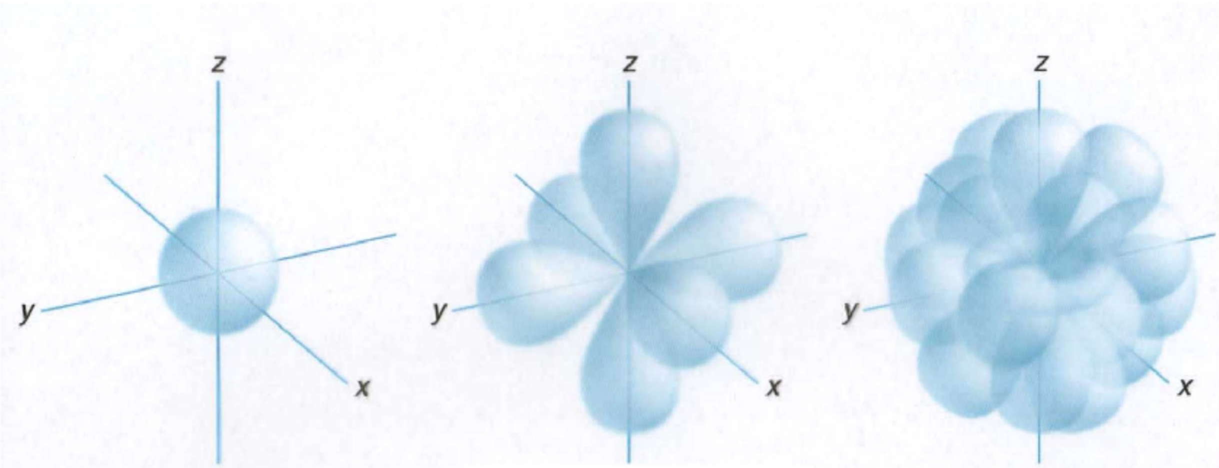
s-orbital

f-orbital

s, p, and d-orbitals



s, p, and d-orbitals



A
s orbitals:
Hold 2 electrons
(outer orbitals of
Groups 1 and 2)

B
p orbitals:
Each of 3 pairs of
lobes holds 2 electrons
= 6 electrons
(outer orbitals of
Groups 13 to 18)

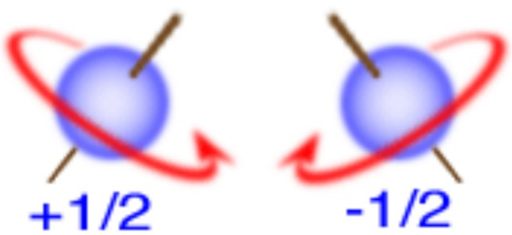
C
***d* orbitals:**
each of 5 sets of
lobes holds 2 electrons
= 10 electrons
(found in elements
with atomic no. of 21
and higher)

D. Spin Quantum Number (m_s)

a. Specifies the direction of the spin of an electron

b. Each orbital can only hold 2 electrons that spin
in opposite directions
(clockwise and counterclockwise)

c. Values for electron spin are +1/2 or -1/2



Pauli Exclusion Principle Again

1. No two electrons in an atom can have the same four quatum numbers.

2. Each electron has a unique "address"

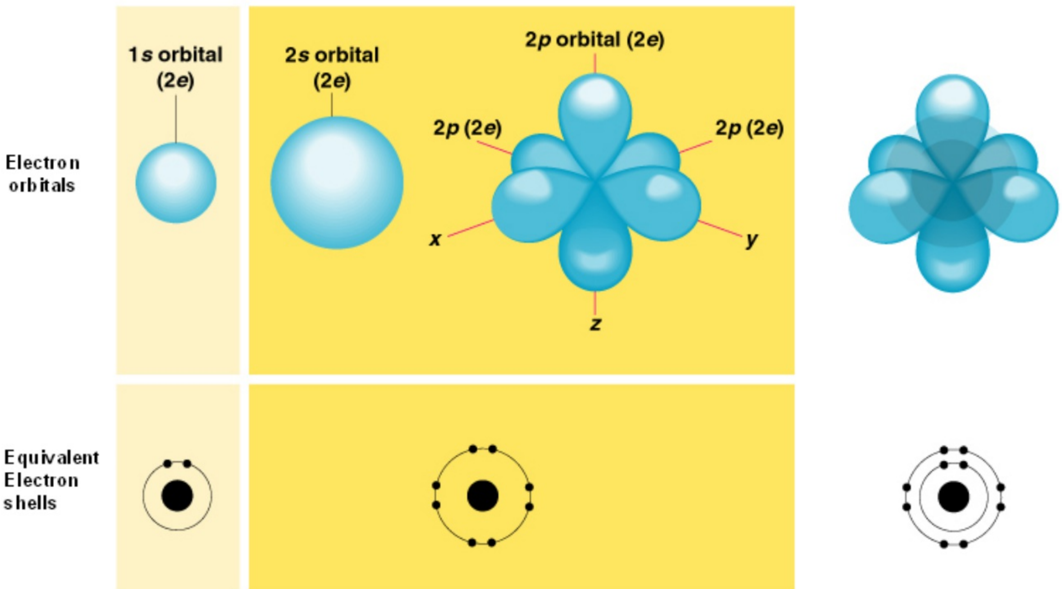
    1. Principle Number --> Energy Level

    2. Angular Momentum # --> sublevel (s,p,d,f)

    3. Magnetic # --> orbital

    4. Spin # --> electron

Electron Orbitals vs. Bohr's Model



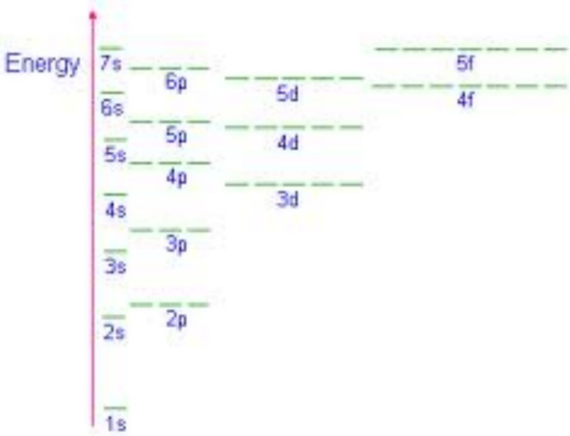
(a) 1s orbital (b) 2s and 2p orbitals c) Neon Ne-10: 1s, 2s and 2p

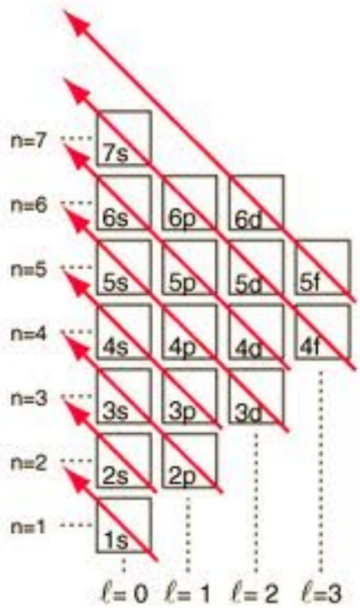
Electron Configurations

1. Electrons follow a set of rules when filling their orbits around a nucleus.

Rules

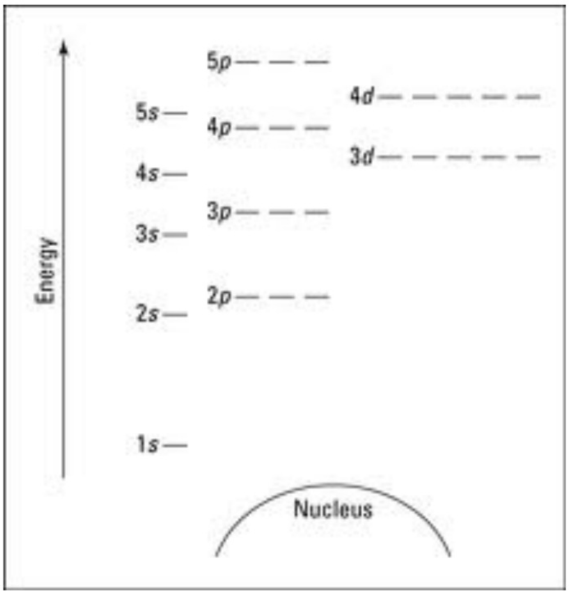
1. **Aufbau Principle**: Electrons are added one at a time to the lowest energy orbitals available until all the electrons of the atom have been accounted for.





1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, etc...

2. **<u>Hund's Rule</u>**: Electrons occupy equal-energy orbitals so that a maximum number of unpaired electrons results.



3. **<u>Pauli Exclusion Principle</u>**: An orbital can only hold a maximum of two electrons. To occupy the same orbital, two electrons must spin in opposite directions.

Maximum Capacities of Subshells and Principal Shells

n	1	2		3			4				...*n*
l	0	0	1	0	1	2	0	1	2	3	
Subshell designation	*s*	*s*	*p*	*s*	*p*	*d*	*s*	*p*	*d*	*f*	
Orbitals in subshell	1	1	3	1	3	5	1	3	5	7	
Subshell capacity	2	2	6	2	6	10	2	6	10	14	
Principal shell capacity	2	8		18			32				...$2n^2$

Hill, Petrucci, General Chemistry *An Integrated Approach* 1999, page 320

When *l* is 0 = s orbit = 1 orbital

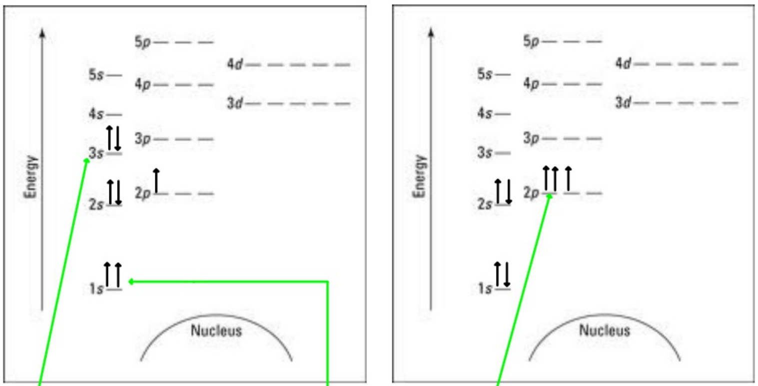
When *l* is 1 = p orbit = 3 orbitals

When *l* is 2 = d orbit = 5 orbitals

When *l* is 3 = f orbit = 7 orbitals

Example: Energy Level Diagram for Nitrogen

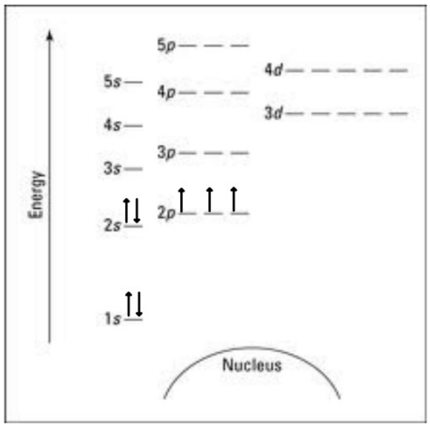
Incorrect



Aufbau Principle and Pauli Exclusion Broke

Hund's Rule Broke

Correct

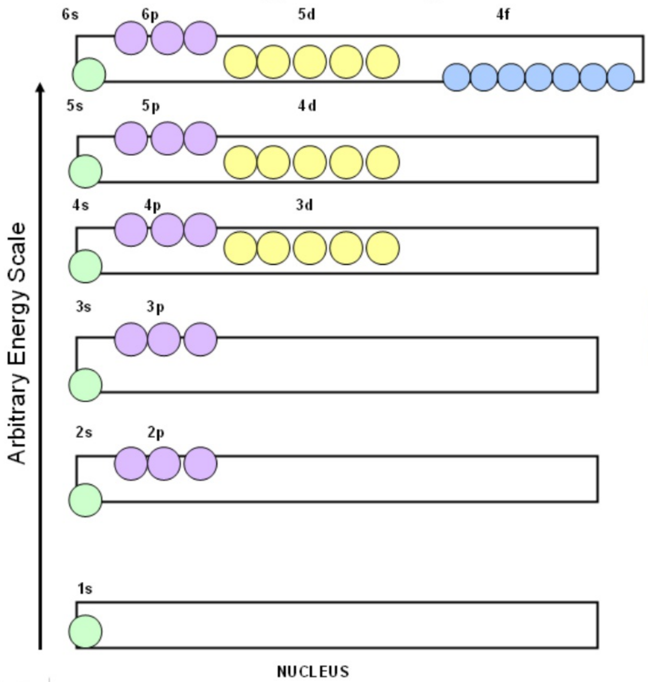


$1s^2\,2s^2\,2p^3$

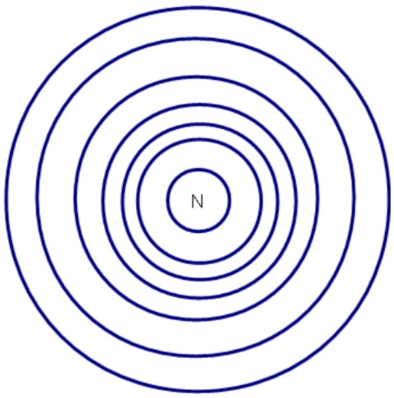
* Arrows pointing up and down represent electrons spinning in opposite directions

* When we write out the electron configuration, you indicate how many electrons are in each sub-level with a superscript.

Energy Level Diagram



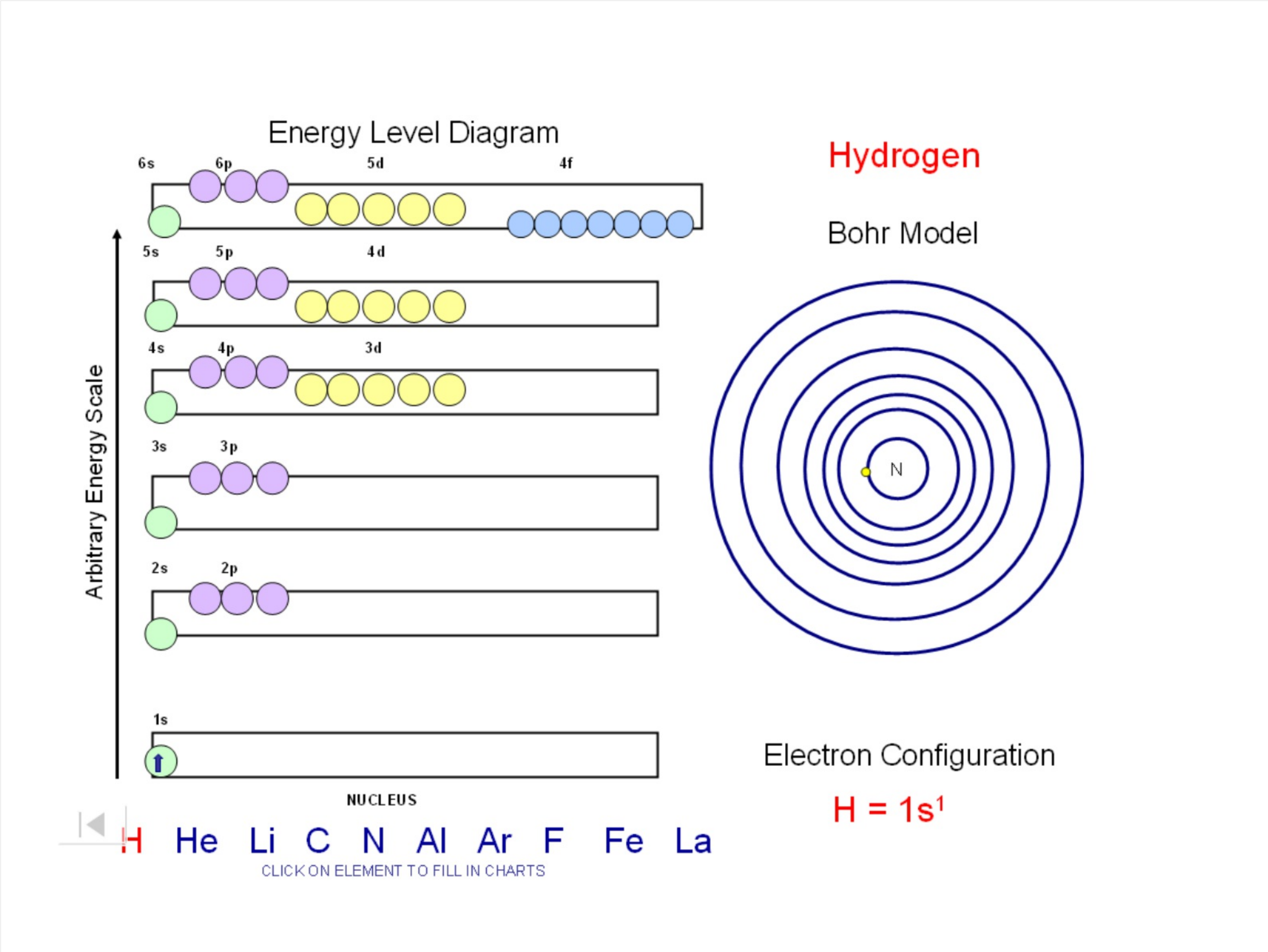
Bohr Model



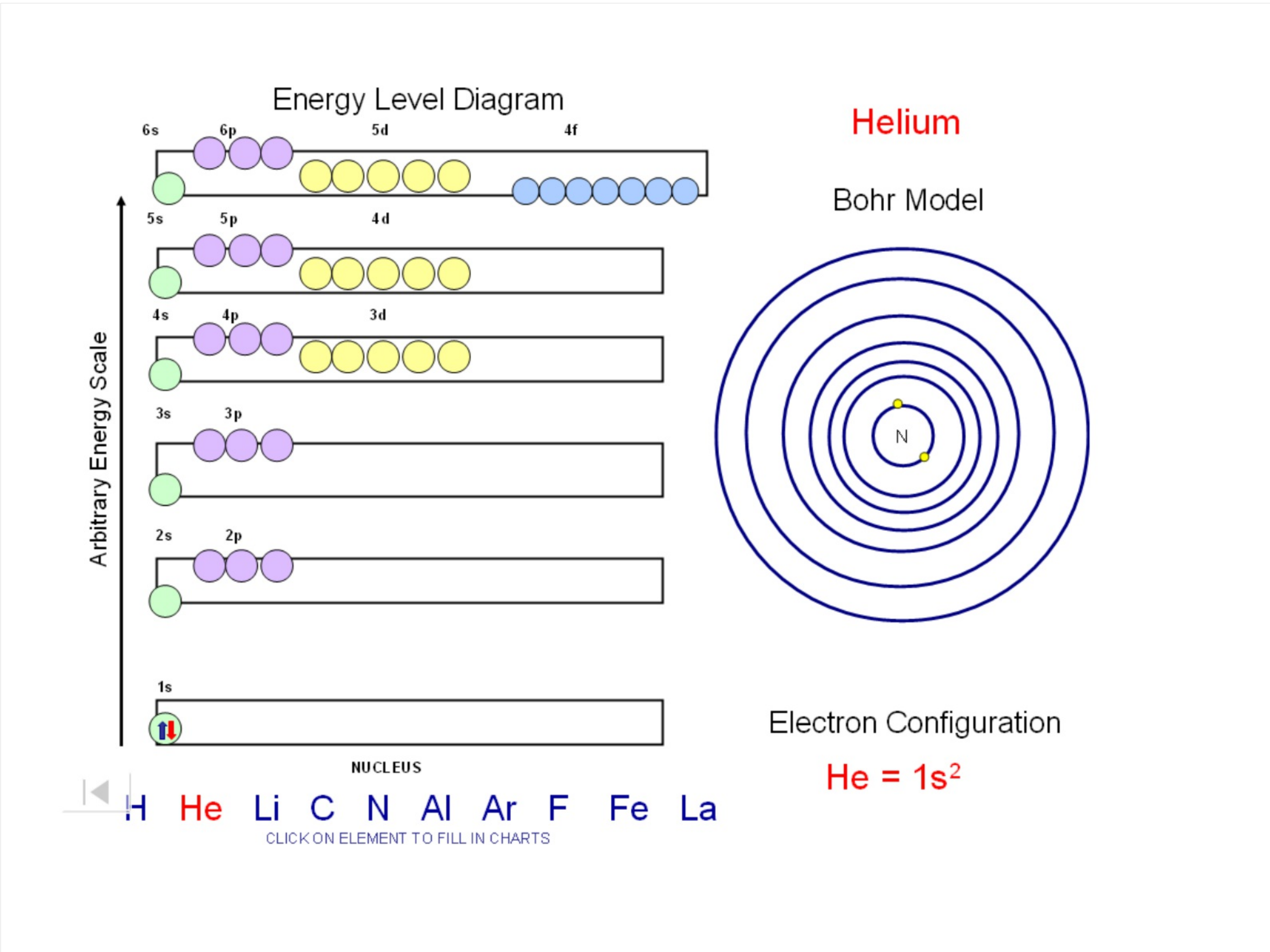
Electron Configuration

H He Li C N Al Ar F Fe La

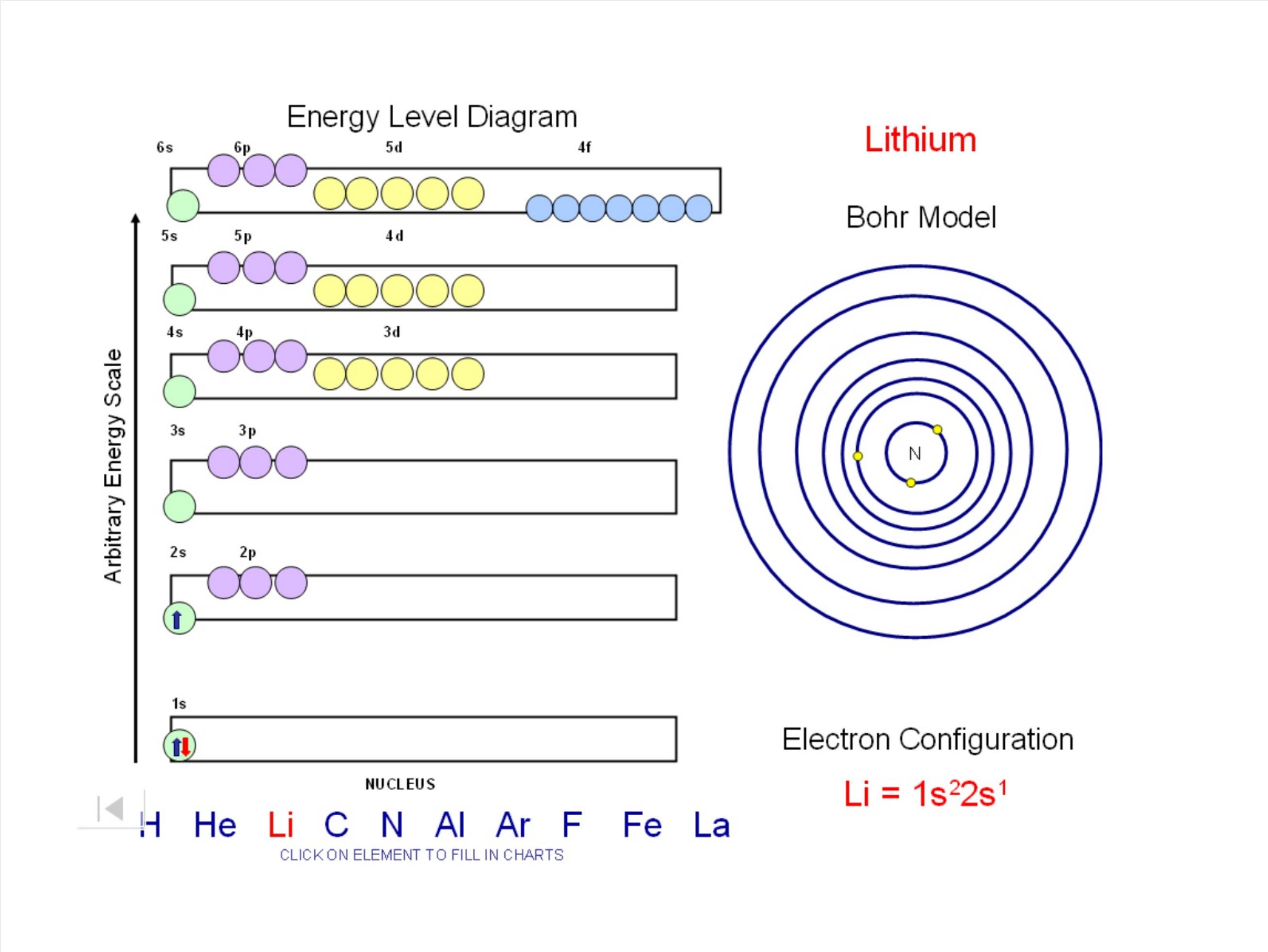
CLICK ON ELEMENT TO FILL IN CHARTS

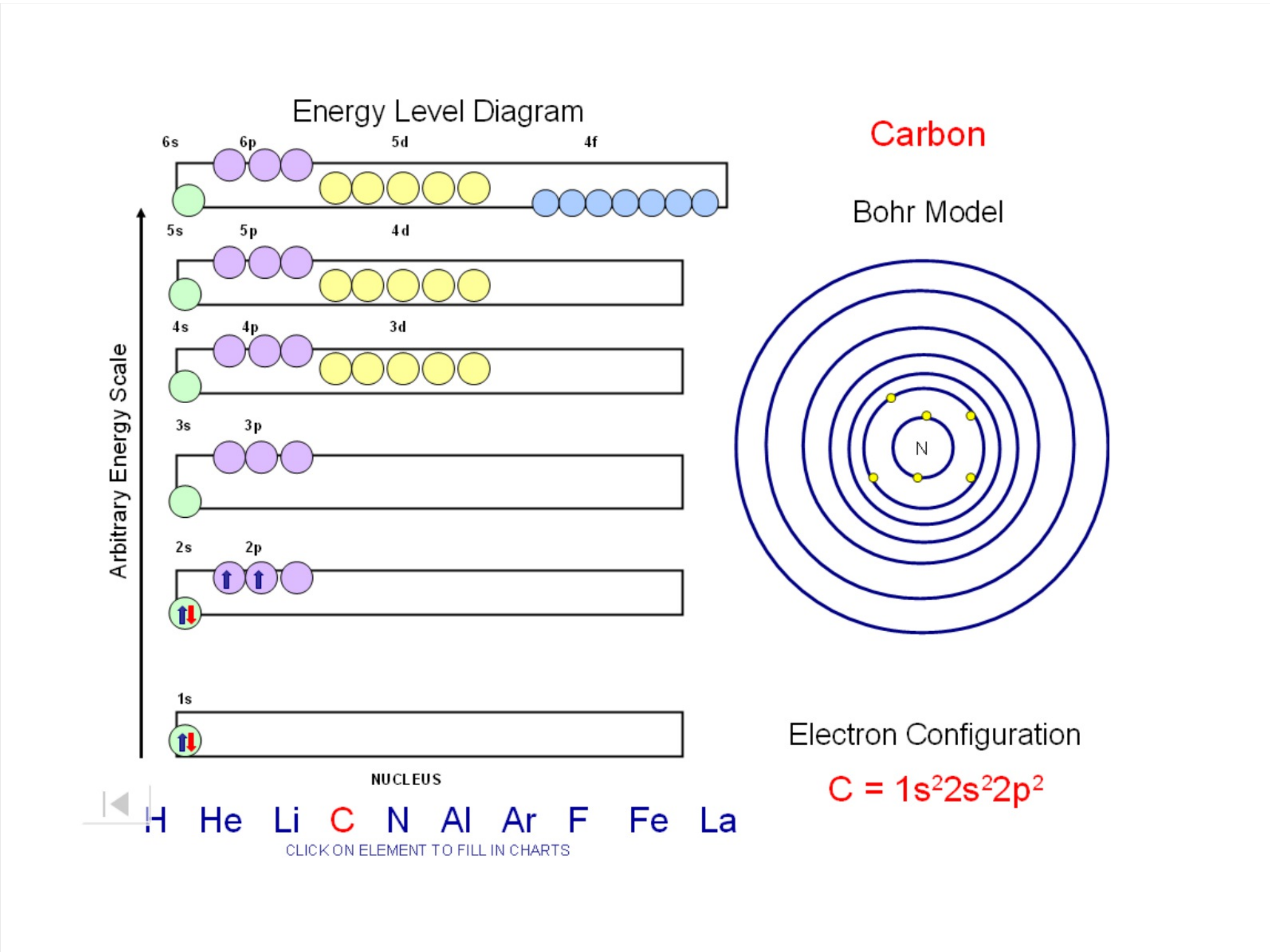


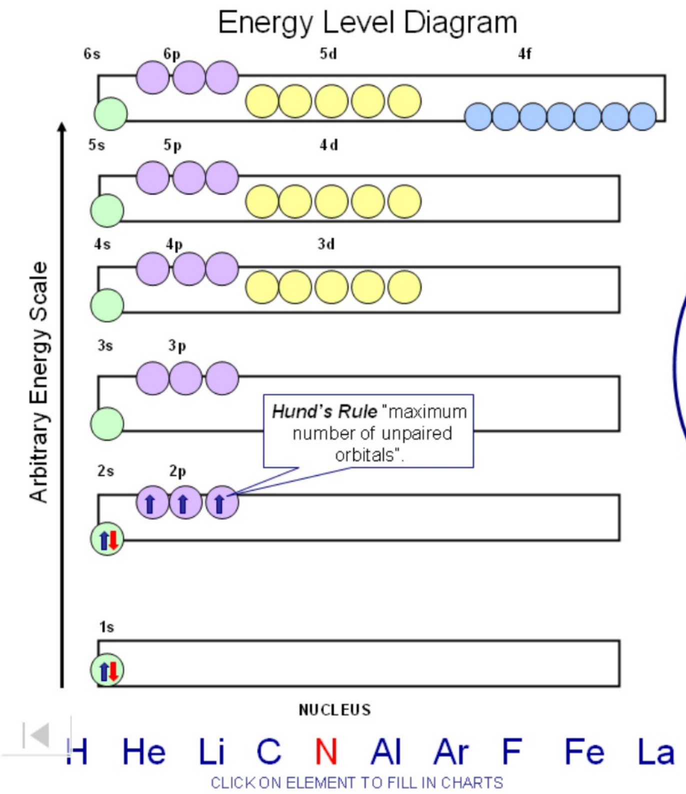
Energy Level Diagram
6s
6p
5d
4f
5s
5p
4d
4s
4p
3d
3s
3p
2s
2p
1s
Arbitrary Energy Scale
NUCLEUS
H He Li C N Al Ar F Fe La
CLICK ON ELEMENT TO FILL IN CHARTS
Hydrogen
Bohr Model
N
Electron Configuration
H = 1s1



Energy Level Diagram
6s
6p
5d
4f
5s
5p
4d
4s
4p
3d
3s
3p
2s
2p
1s
Arbitrary Energy Scale
NUCLEUS
H He Li C N Al Ar F Fe La
CLICK ON ELEMENT TO FILL IN CHARTS
Helium
Bohr Model
N
Electron Configuration
He = 1s2

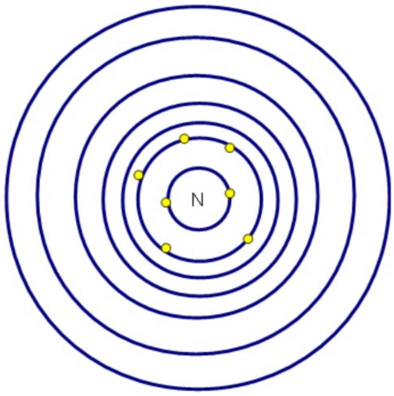

Energy Level Diagram
6s
6p
5d
4f
5s
5p
4d
4s
4p
3d
3s
3p
2s
2p
1s
Arbitrary Energy Scale
NUCLEUS
H He Li C N Al Ar F Fe La
CLICK ON ELEMENT TO FILL IN CHARTS
Lithium
Bohr Model
N
Electron Configuration
Li = 1s22s1


Energy Level Diagram
6s
6p
5d
4f
5s
5p
4d
4s
4p
3d
3s
3p
2s
2p
1s
Arbitrary Energy Scale
NUCLEUS
H He Li C N Al Ar F Fe La
CLICK ON ELEMENT TO FILL IN CHARTS
Carbon
Bohr Model
N
Electron Configuration
C = 1s22s22p2



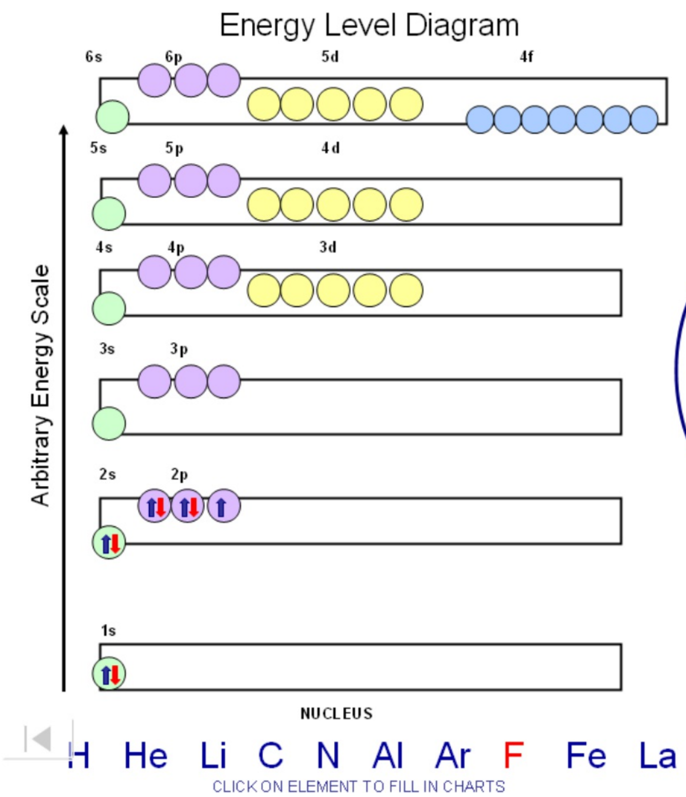
Nitrogen

Bohr Model



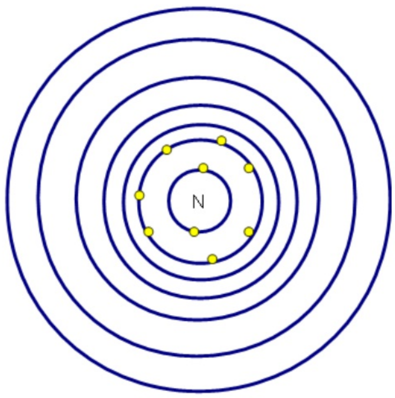
Electron Configuration

$N = 1s^2 2s^2 2p^3$



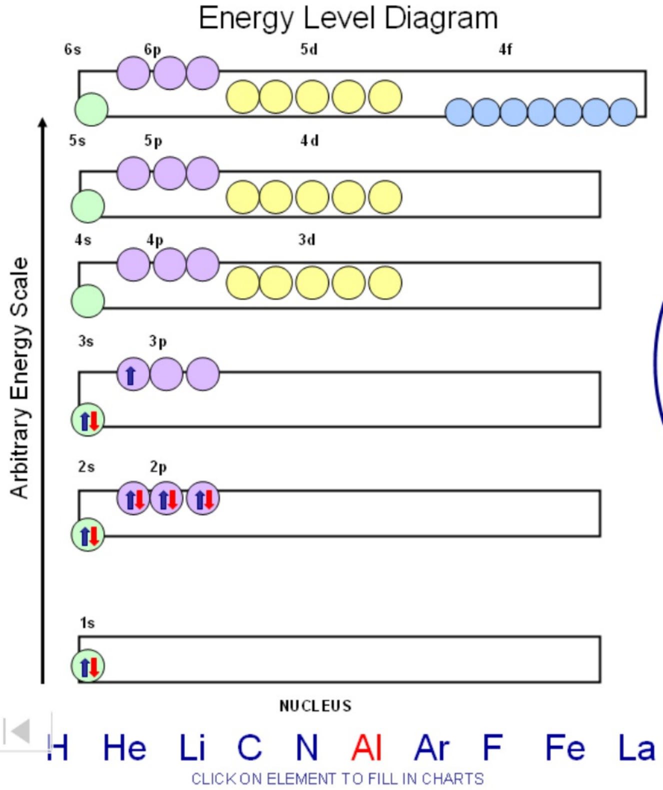
Fluorine

Bohr Model



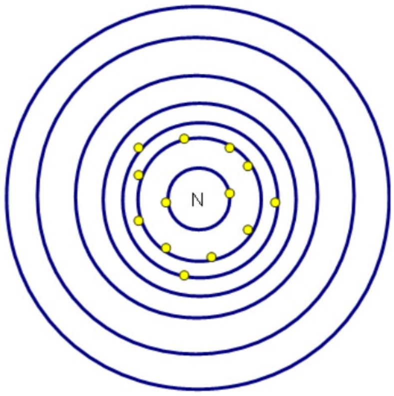
Electron Configuration

$F = 1s^2 2s^2 2p^5$



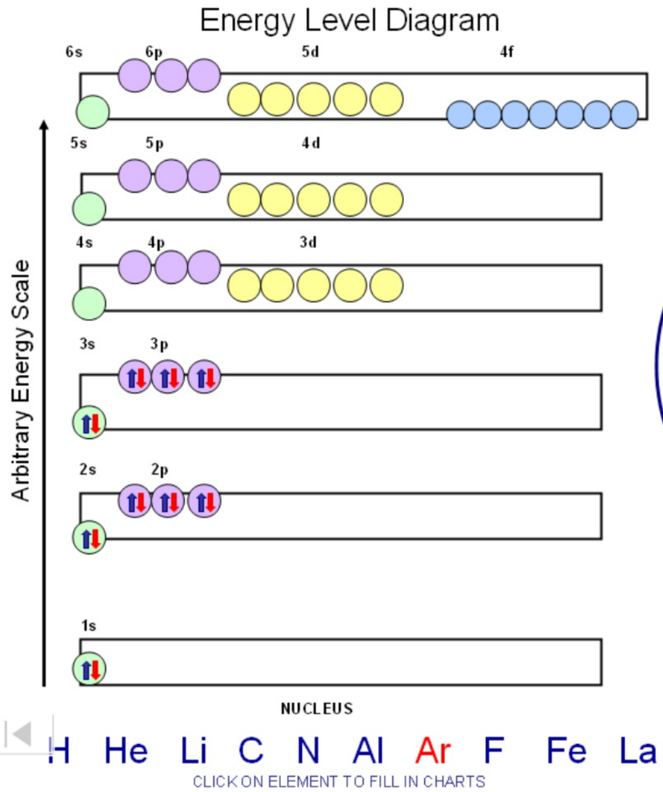
Aluminum

Bohr Model



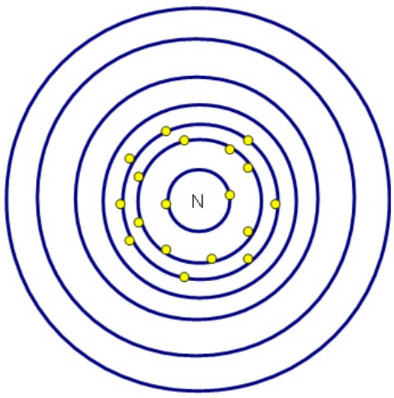
Electron Configuration

Al = $1s^2 2s^2 2p^6 3s^2 3p^1$



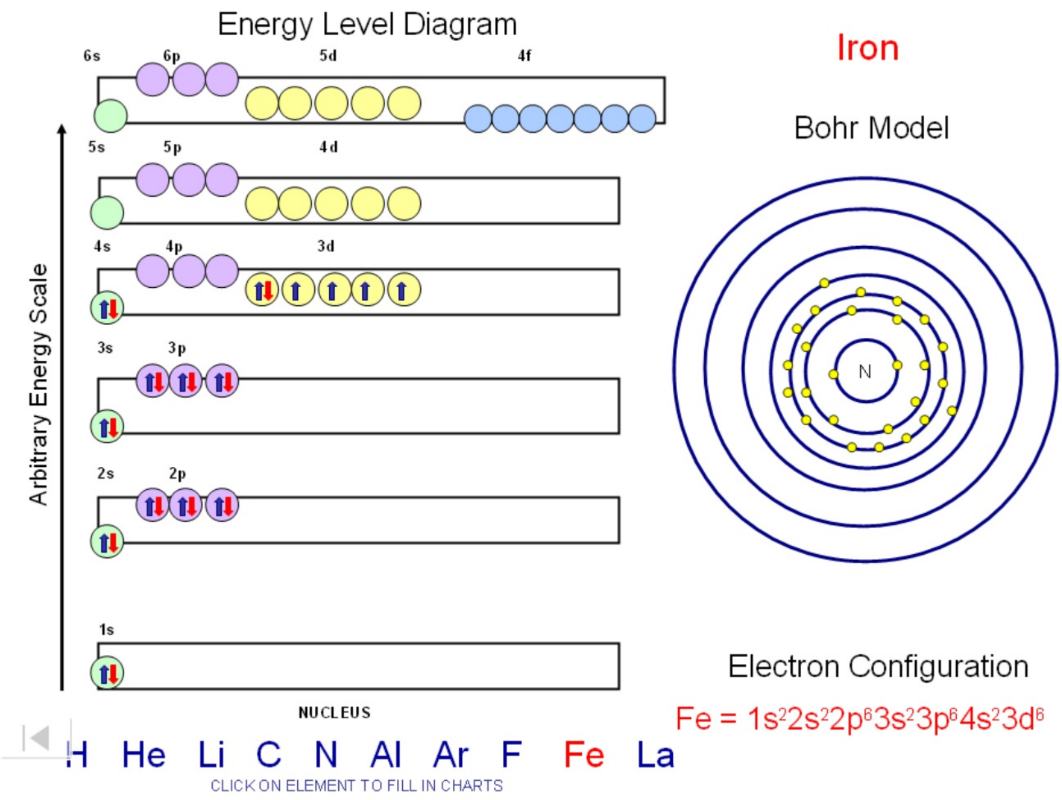
Argon

Bohr Model



Electron Configuration

Ar = $1s^2 2s^2 2p^6 3s^2 3p^6$



<u>Shorthand Electron Configuration (Noble Gas Config.)</u>

1. This is yet another way to write electron configurations.

2. This is a shorter, quicker way to write them.

3. To write a S.E.C.

   A. Put symbol of noble gas that precedes element in brackets.

   B. Continue writing electron config. from that point.

Examples:

Sulfur (S)

[Ne] $3s^2 3p^4$

Cobalt (Co)

[Ar] $4s^2 3d^7$

Calcium (Ca)

[Ar] $4s^2$

Iodine (I)

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

Periodic Patterns