Early atomic theory

Atomic mass

- **Base mass is carbon 12 with an AMU of 12 and 12 grams/mole**
- **An *ATOMIC MASS UNIT* *(AMU)* is 1/12 the mass of Carbon**
- **Average atomic mass**

Isotopes and atomic numbers

- **Isotopes have the same # of protons but different numbers of neutrons**
  - **The atomic number (Z) is equal to the number of protons in the nucleus of an element**
  - **Nucleus is the center of the atom made up of protons and neutrons**
  - **Mass number (A) is equal to the number of protons plus the number of neutrons**
  - **Nucleons – are particles that make up the nucleus of the atom (protons and neutrons)**
  - **Nuclide - a particular kind of atom containing a definite number of protons and neutrons**
  - **Number of Neutrons = A - Z**

mass spectrometer measures the mass amounts of isotopes

- **Isotope Mass Fractional abundance**

  Cr - 50 49.946 4.35%=2.1727
  Cr - 52 51.941 83.8%=43.527
  Cr - 53 52.941 9.5% =5.0294
  Cr - 54 51.996 2.35%=1.2219

  51.996

- **Each isotope mass is multiplied by its fractional abundance**

Democritus 400 BC

- **World made of Two things**
  a. **Empty space**
  b. **Atoms (tiny particles)**

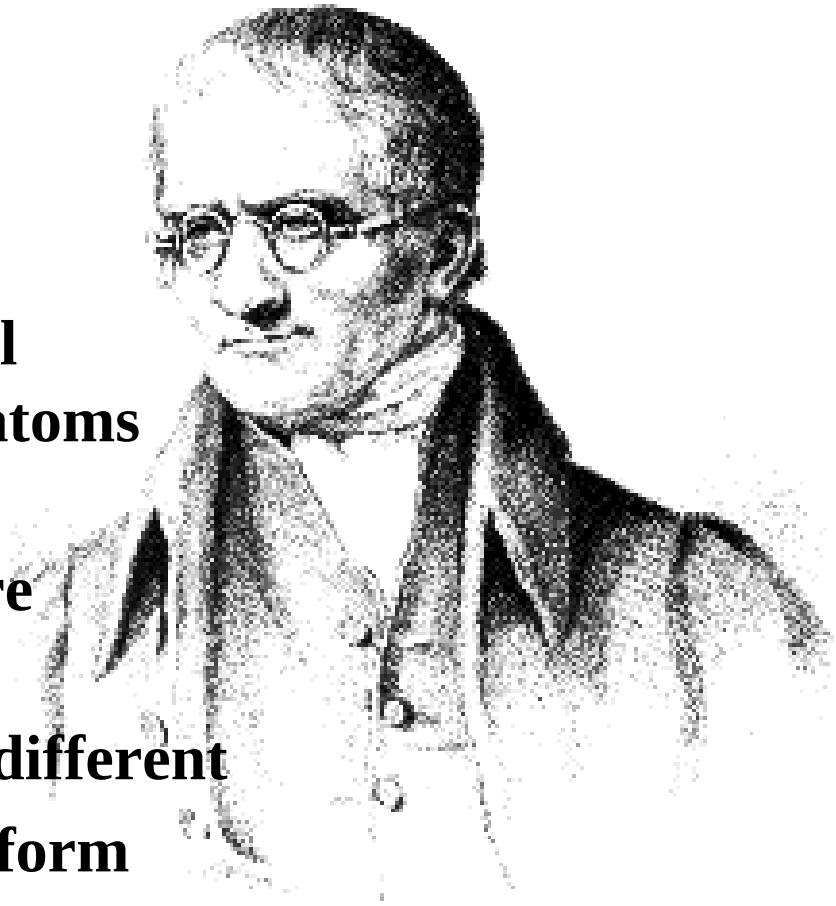
Antoine Lavoiseir (1800)

- **In a closed system mass before a reaction is equal to mass after the reaction**
- **Matter can be changed in many ways but cannot be created or destroyed**
  - **Law of conservation of mass**

Joseph Proust

- **(Law of definite composition) elements in a substance have definite proportions by mass**

Dalton's Theory



- **Four things**
  - **Matter is composed of very small particles called atoms and these atoms can't be broken apart**
  - **All atoms of the same element are identical**
  - **Atoms of different elements are different**
  - **Atoms unite in definite ratios to form compounds**
    - **Law of multiple proportions - The ratio of masses of one element that combine with a constant mass of another element can be expressed in small whole numbers**

J.L. Gay Lussac

- **noted that under constant temperature and pressure volumes of reacting gases and gas products were in ratios of small whole numbers**

Avogadro

- **equal volumes of gas under the same conditions have the same number of molecules**

Early research on Atomic Particles

Millikan

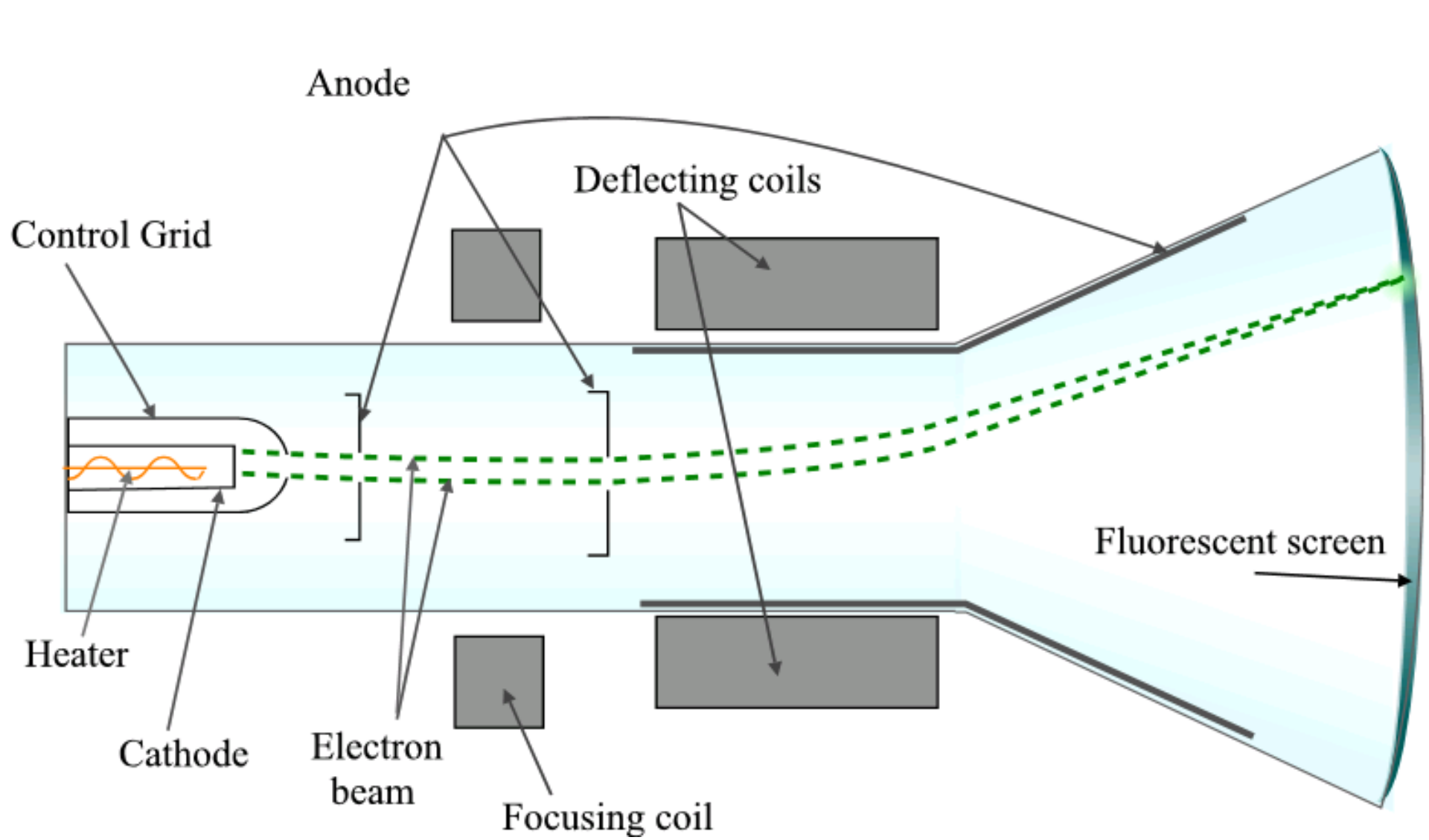
- **first to discover the charge of an electron**
  - **Electron ē**

Cathode ray tube (JJ Tompson 1897)

J.J. Thompson

- Each end is an electrode
  - Positive terminal - anode
  - Negative terminal - cathode
- Cathode rays are streams of electrons
- Thompson measured the bending of the path of cathode rays and was able to determine the ratio of electron charge to its mass

- By using m x v = momentum and forces


Anode
Deflecting coils
Control Grid
Fluorescent screen
Heater
Cathode
Electron beam
Focusing coil

Thompson

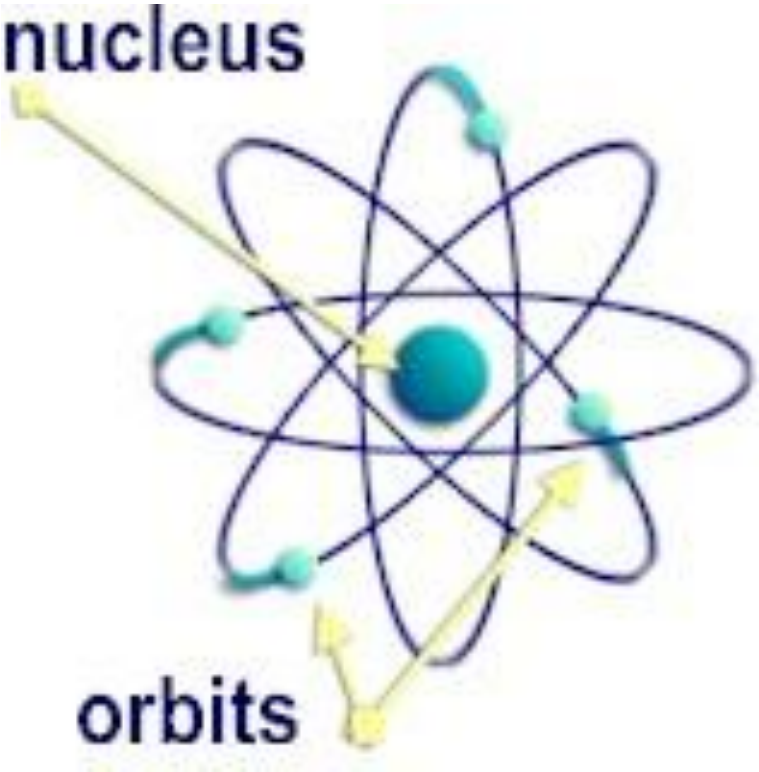
- **found protons to have the same charge as electrons only opposite and to have a mass of 1836 times that of an electron**

James Chadwick

- **discovered a particle with no charge and essentially the same mass of a proton** (neutron)

Rutherford/Bohr Atom

- **Experiments showed that the atom has a central positive center surrounded by electrons**



Geiger and Marsden subjected

- **Thin sheet of gold to alpha particles (protons)**
- **Most of the particles passed through**
- **Some were deflected and some bounced back**
- **Atoms are mostly empty space, so why did some bounce back or were deflected**

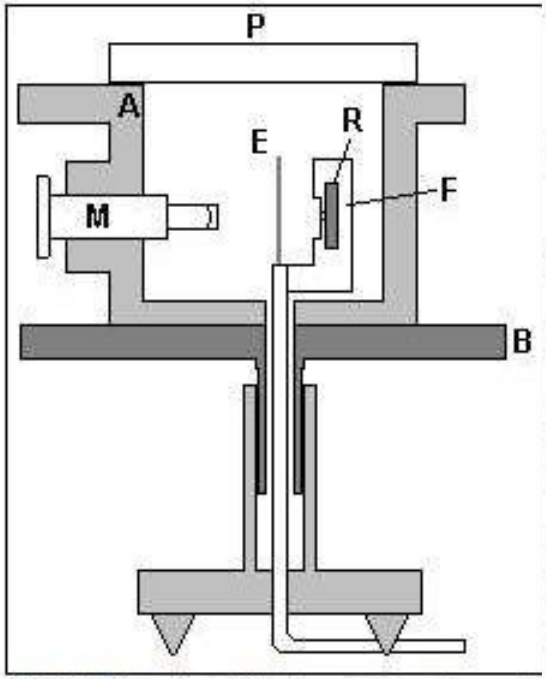
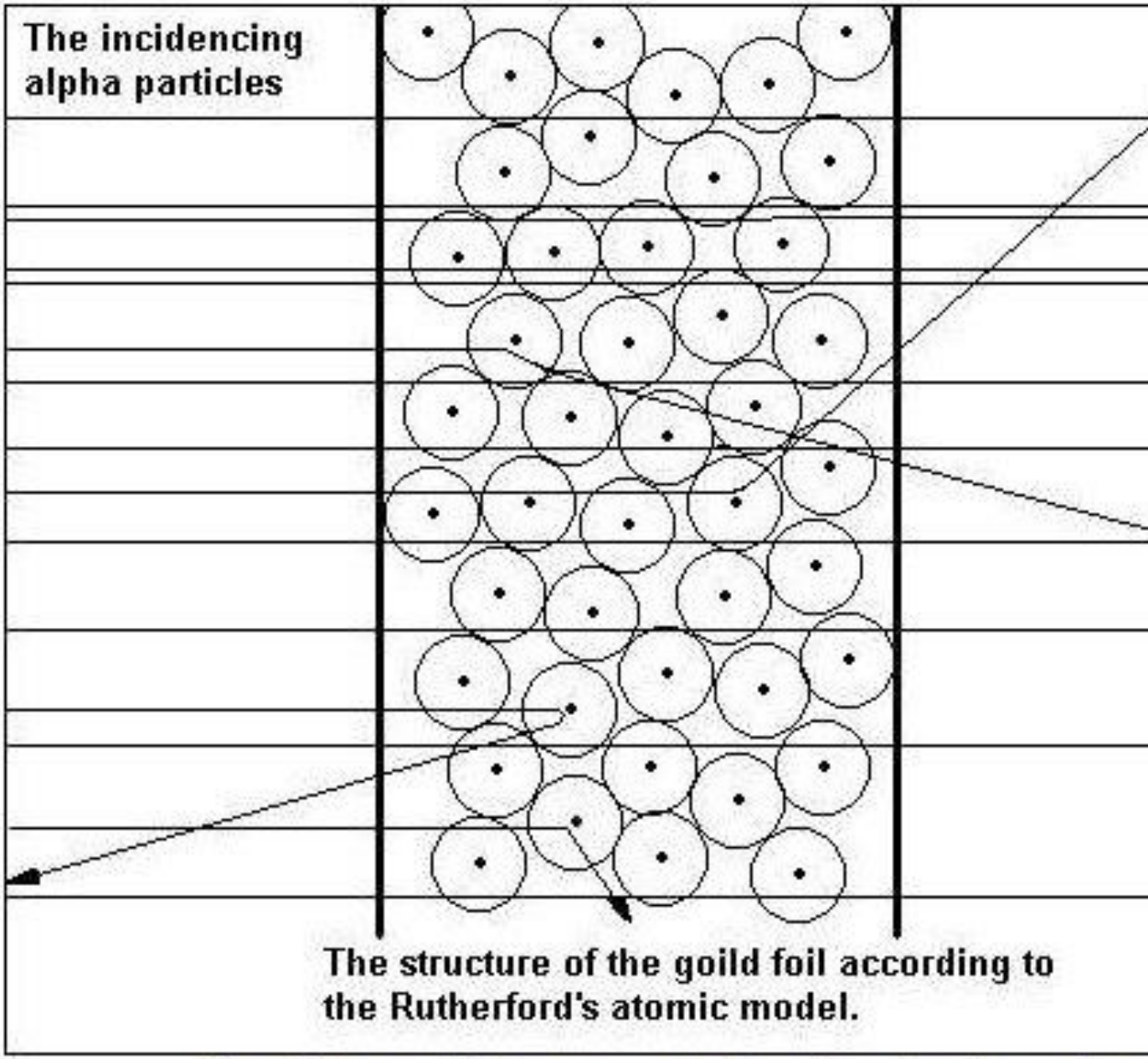


Fig1. Marsden-Geiger experiment.



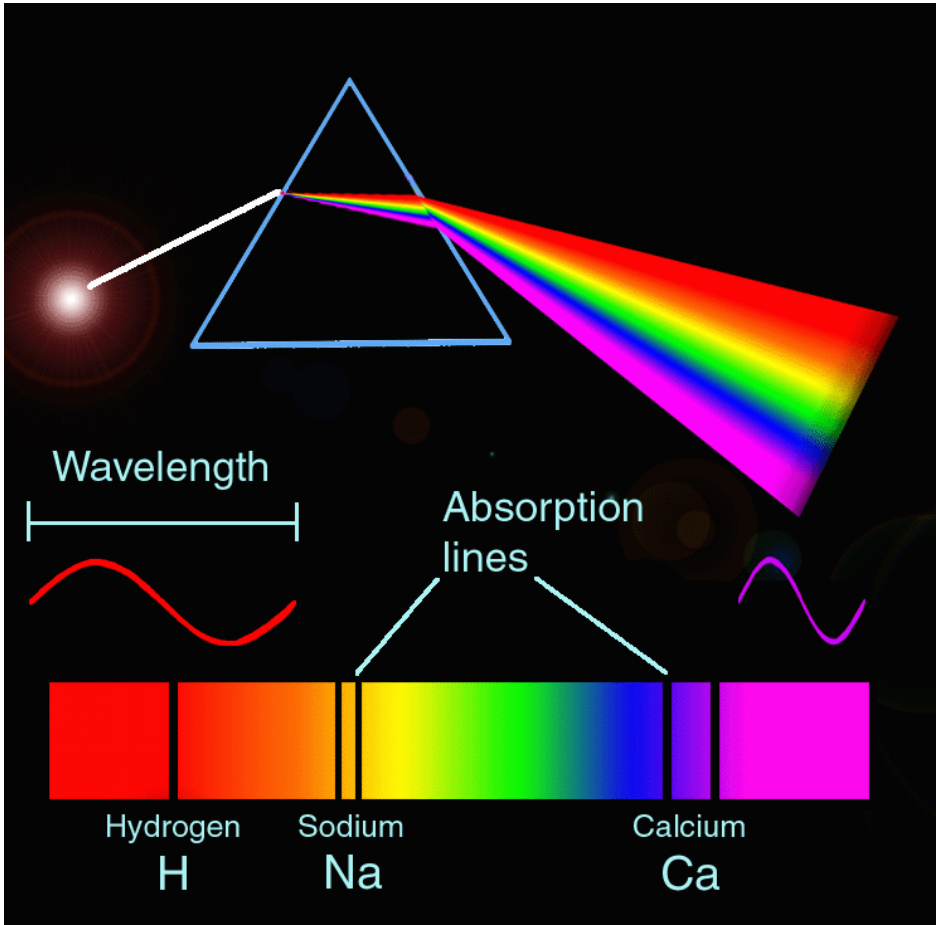
The alpha particles propagated on the atomic nucleus

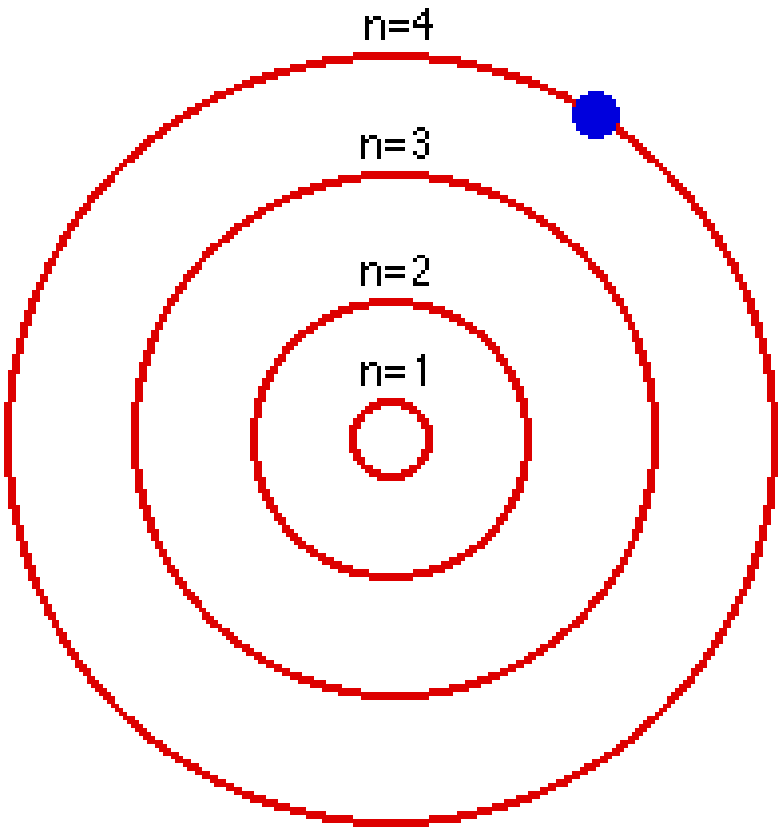
Hydrogen Atoms

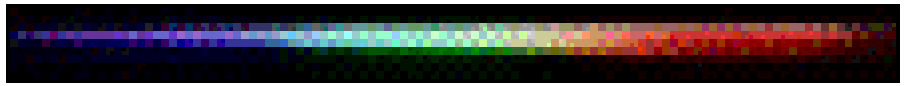
- **Using a model of a hydrogen atom with a ping pong ball being the nucleus and the electron the same size they would be 1.35 km apart**
- **Planetary model - electrons orbit the nucleus like planets around the sun**

Spectroscopy

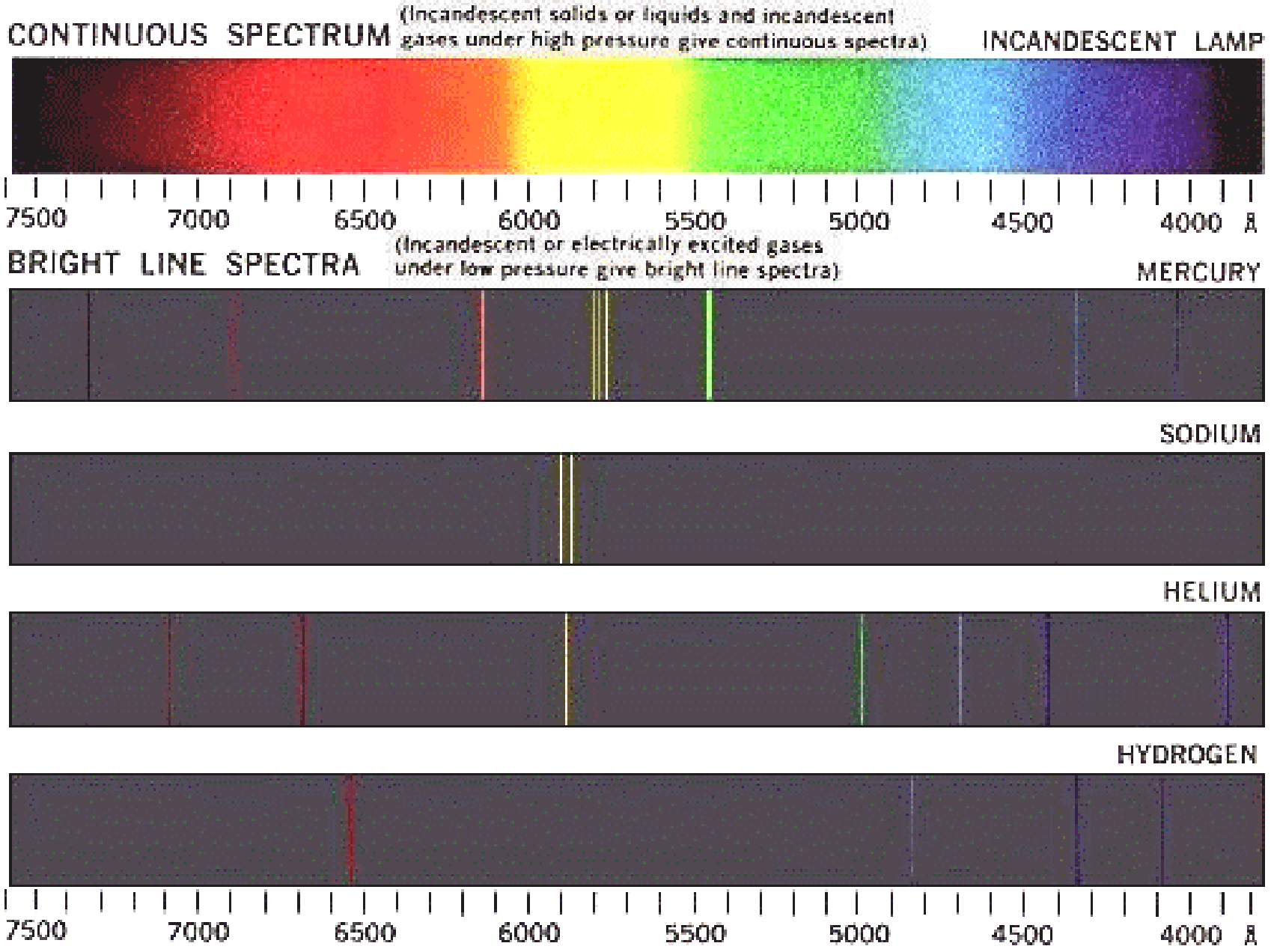
- **Method of studying substances that are exposed to some sort of continuous excited energy**
  - **Atoms absorb energy**
  - **Light is emitted from the atom when electrons return to the "ground state"**




n=4
n=3
n=2
n=1



EMISSION SPECTRA



Electromagnetic energy -

- **Energy that consists of variation in electric and magnetic fields.**
  - **Frequency (v) is measured in hertz (Hz) Waves/Second**
  - **Velocity is m/s (v)**
    - **Speed of light is (c) 3.00 x 10^8 m/s**
  - **Wavelength (λ) distance from crest to crest to crest or trough to tough**
  - **Amplitude – maximum displacement from rest**

Plank's Hypothesis

- **Quantum theory – Concept that energy is given off in discrete packets rather than continuously**
- **These little quanta or packets are called photons**
- **Amount of energy given off is related to frequency**
  - **$E = h \nu$**
  - E=Energy
  - **h = Plank's constant = 6.6262 x 10^{-34} J/Hz**
  - **ν = frequency, so velocity/wavelength=frequency**
  - or C (speed of light) = λν
  - to get E= h (c/λ)
  - **The greater the frequency the greater the energy**

Hydrogen Atom quantum theory

- **Energy wavelength corresponds to a definite change in the energy of an electron**
- **Electrons absorb and emit only whole number of quanta (photons)**
- **When electrons drop from a larger orbit to a smaller one, energy is emitted.**
- **ground state level has the least energy**
- **$\lambda = c/\nu$ & $E = h\nu$**
- **Photoelectric effect - emission of electrons from certain substances when exposed to light of suitable of suitable frequency**

Electron Cloud Probability

DeBroglies Hypothesis

- **Suggested that particles have characteristics of waves**

1. He used both Einstein's and Plank's theories

a. $E = mc^2$ and $E = h \nu$

b. Then $mc^2 = h \nu$

c. $\nu = v/\lambda$

d. $mv = p$, then $\lambda = h/mv$ (p = momentum)

e. $p = h/\lambda$, $\lambda = h/p$

f. So as momentum increases wave length decreases

E. The apparent contradiction

1. Light travels at different speeds in different substances and is bent when it enters a different substance like it is particles traveling in a straight line or beam

2. Light shows behaviors of interference like a wave.

3. It is both a wave and a particle

Newtonian mechanics –

- **describes the behavior of visible objects traveling at ordinary velocities**
  (The big slow world)

Quantum mechanics -

- **describes the behavior of extremely small particles traveling at velocities near the speed of light**
  (The Small Fast World)

Measuring momentum and position of electrons

- **Heisenbergs principle - The exact position and momentum of an electron cannot be determined at the same time.**

Schrodingers work -

- **examines the electron as a wave, not a particle**
- **Found the probability of finding an electron in a certain area**
  - **This gave an address or an approximate location of an electron around the nucleus of the atom**
  - **Quantum numbers describe what is called the electron probability**

Quantum numbers represent different energy states of the electrons

- There are four quantum numbers (n,l,m &s)
  - Principle – n – energy level
  - Second – l – sub energy level
  - Third – m – orbital
  - Fourth – s – describes the spin

Principle quantum number

- **represents the energy level of the electron (1,2,3 . .)**
  - **The total number of electrons in an energy level $2n^2$**

Quantum Numbers

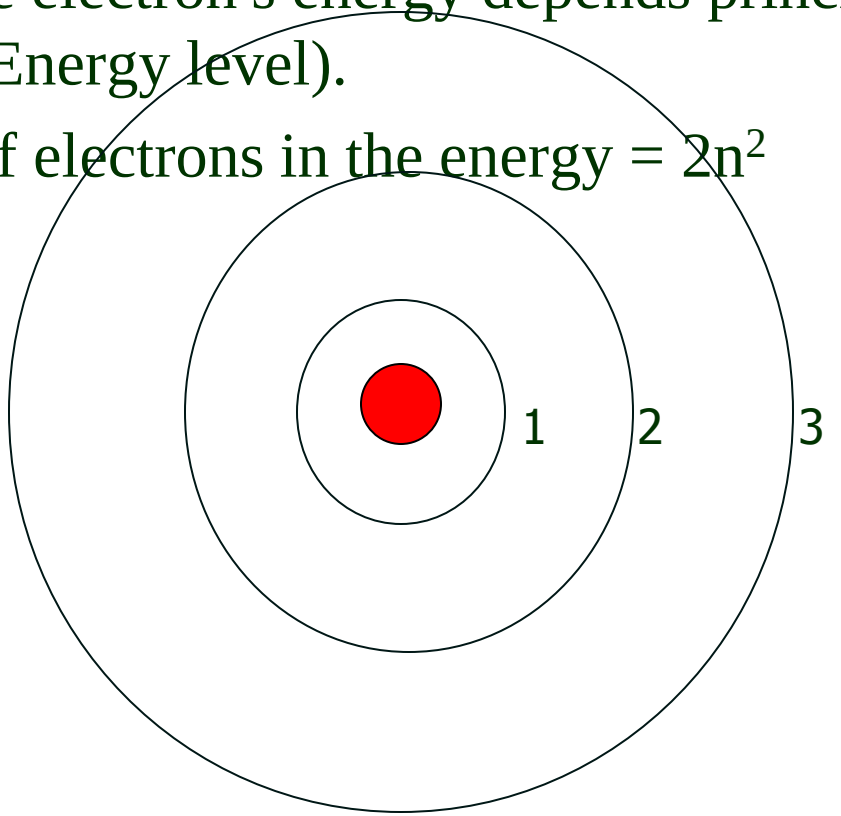
- The principal quantum number has the symbol n.

  n = 1, 2, 3, 4, ... "shells"

  (n = K, L, M, N, ...)

  The electron's energy depends principally on n (Energy level).

  # of electrons in the energy = $2n^2$



The second quantum number (l)

- **Describes the sub energy levels**
  - **Each energy level has sublevels equal to its number**
  - **The sublevels are s,p,d & f**

Orbital Angular Momentum (l)

Specifies the subshell the electron occupies l =0, 1,...(n-1), also referred to as states s, p, d, f

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

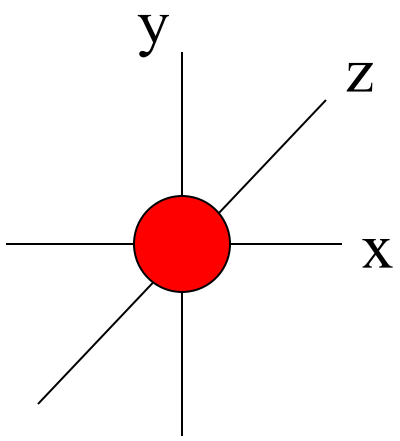
Third quantum number (m)

- **Describes orbitals**
  - **Orbitals are the space occupied by a pair of electrons**
  - **Describes the orientation in space of each orbital**
  - **The number of orbitals is equal to the number of pairs of electrons in a sublevel** (2 electrons/orbital)

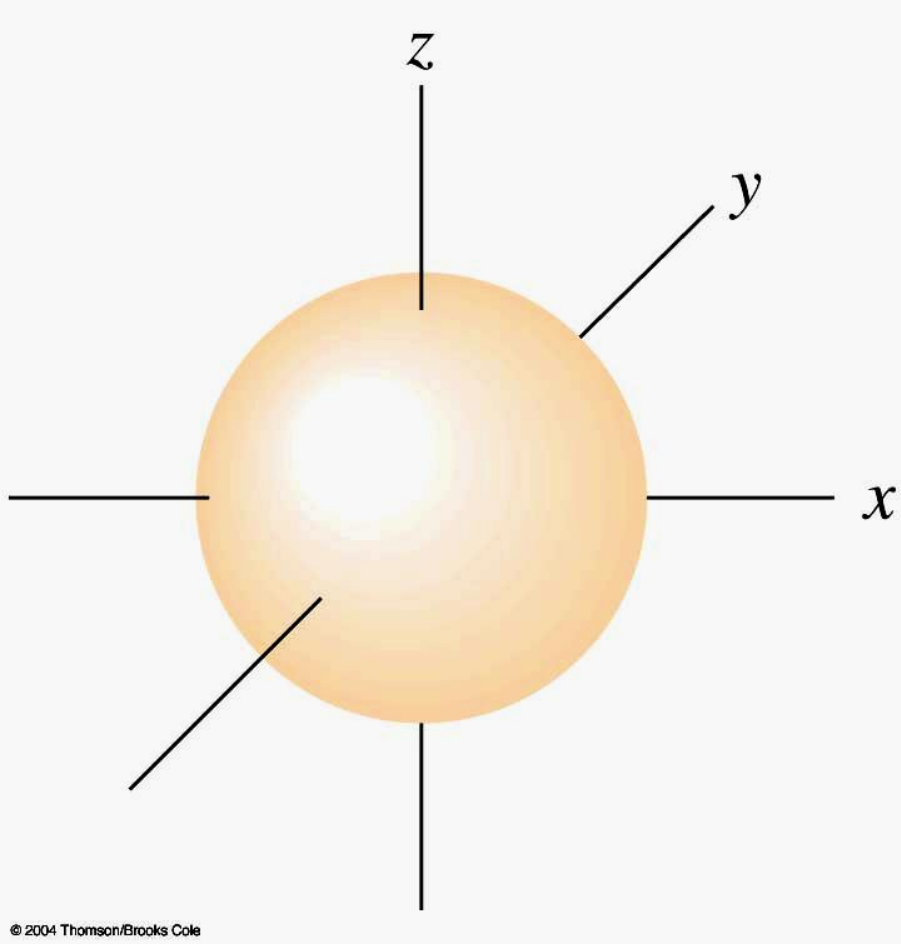
s sublevel	**1 orbital**
p sublevel	**3 orbitals**
d sublevel	**5 orbitals**
f sublevel	**7 orbitals**

Quantum Numbers

- The third quantum # m**, represents the spatial orientation.**
- Atomic orbitals are regions of space where the probability of finding an electron about an atom is highest.



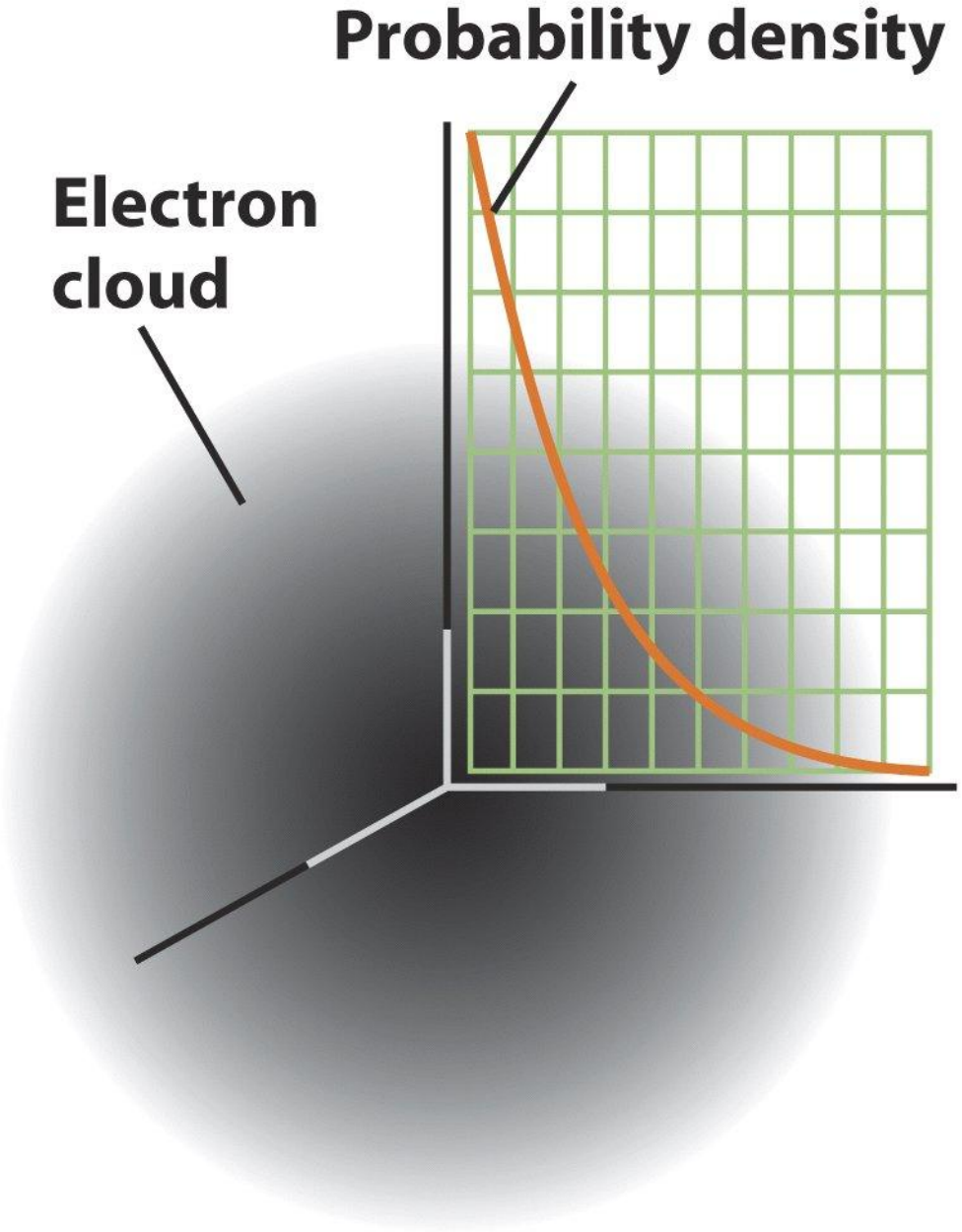
- s orbitals are spherically symmetric



For every s orbital:

$\ell = 0$ and $m_\ell = 0$

The only thing that changes for s orbitals is n.



1s orbital of hydrogen

p orbitals

- p orbital properties:
  - The first p orbitals appear in the n = 2 shell.

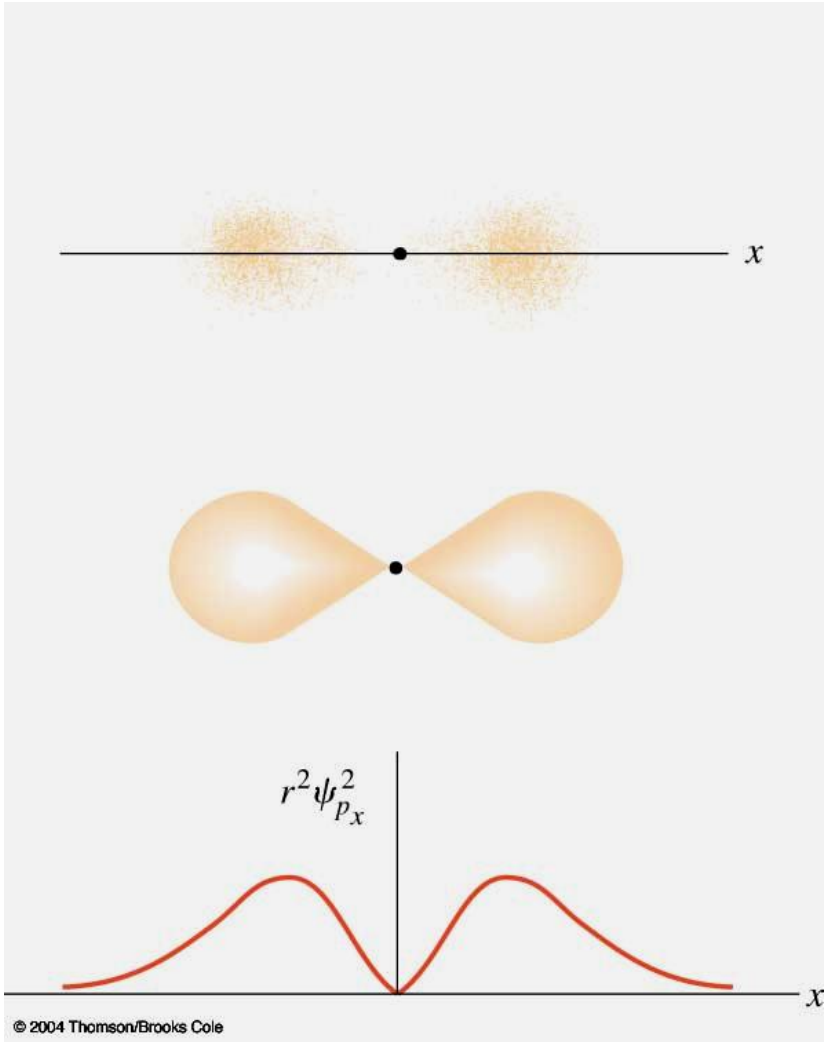
- p orbitals are peanut or dumbbell shaped volumes.

- There are 3 p orbitals per n level.
  - The three orbitals are named p_x, p_y, p_z.

  $\ell = 1$ for all p orbitals.

  m_ℓ = -1,0,+1 (designate the three orientations)

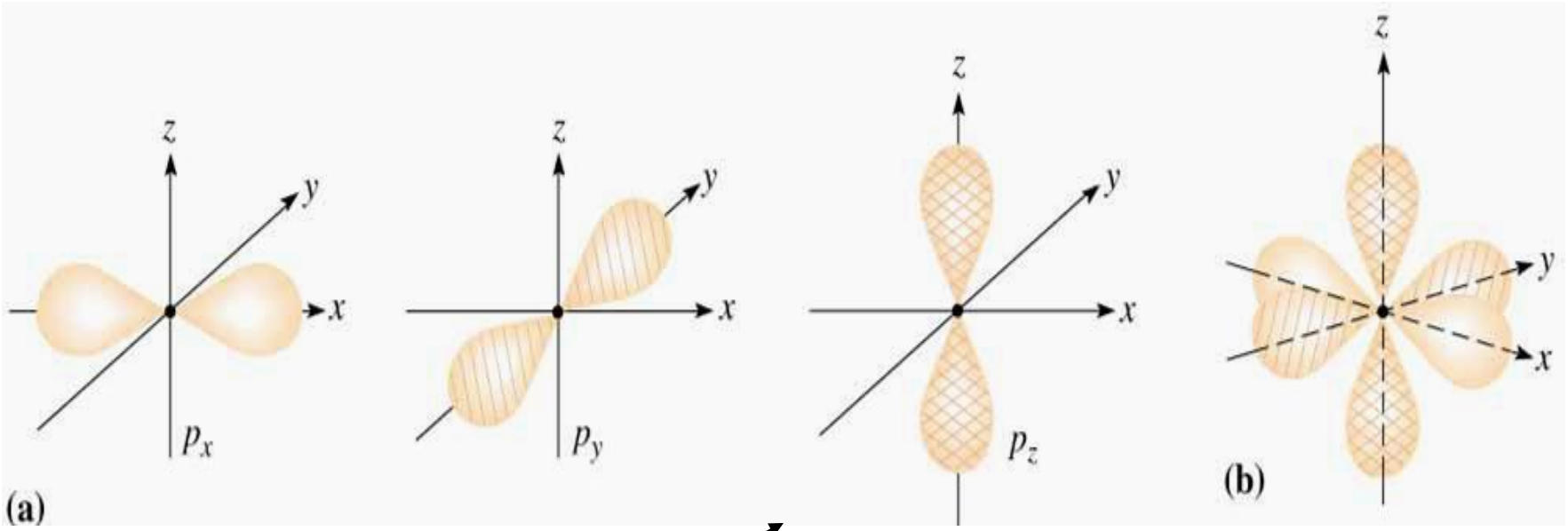
- p orbitals are peanut or dumbbell shaped.



$\ell = 1$

- p orbitals are peanut or dumbbell shaped.

$\ell = 1$



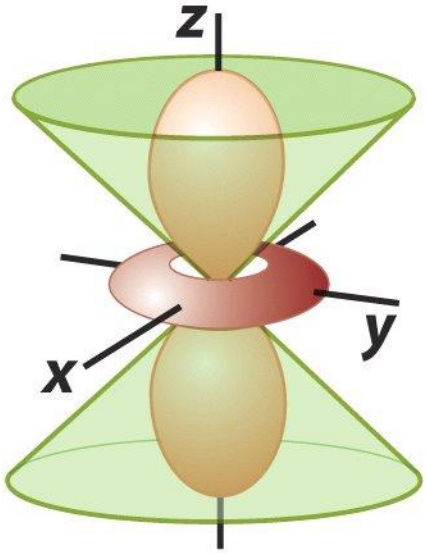
$m_\ell = -1,0,+1$

d orbital properties:

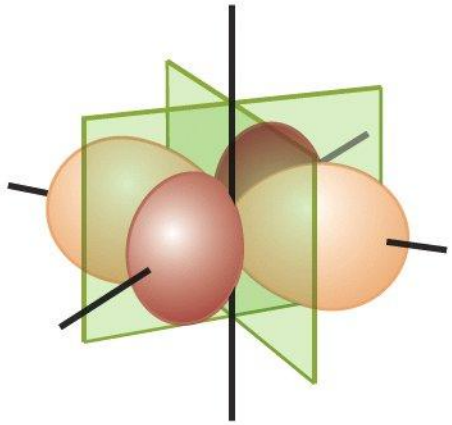
- The first d orbitals appear in the n = 3 shell.

- The five d orbitals have two different shapes:
  - 4 are clover leaf shaped.
  - 1 is peanut shaped with a doughnut around it.
  - The orbitals lie directly on the Cartesian axes or are rotated 45^{o} from the axes.

- There are 5 d orbitals per n level.
  - The five orbitals are named: $d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$
  - They have an $\ell = 2$.
  - $m_\ell = -2,-1,0,+1,+2$ (5 values of m_ℓ)



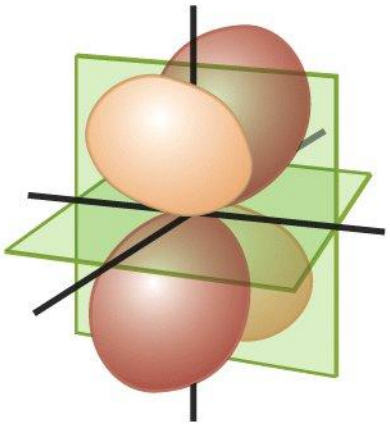
d_{z^2}



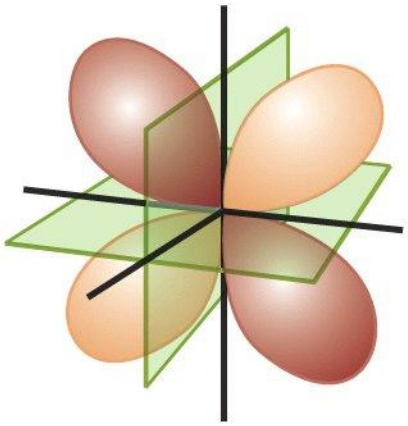
$d_{x^2-y^2}$

$\ell = 2$

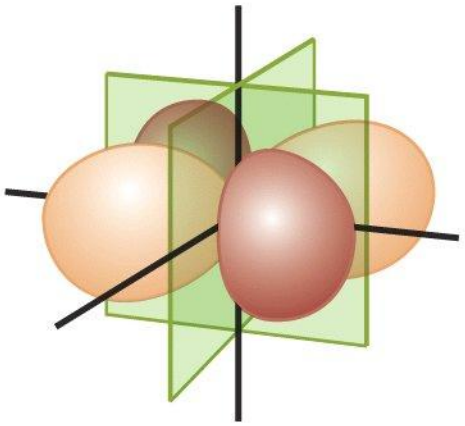
m_ℓ = -2,-1,0,+1,+2



d_{zx}



d_{yz}



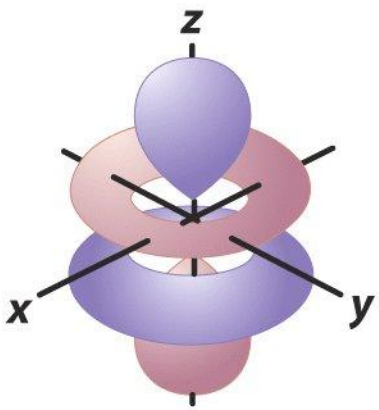
d_{xy}

f orbital properties:

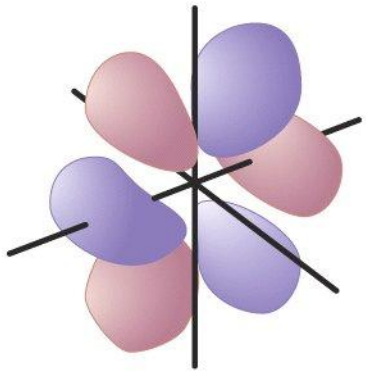
- The first f orbitals appear in the n = 4 shell.
- The f orbitals have the most complex shapes.
- There are seven f orbitals per n level.
  - The f orbitals have complicated names.
  - They have an $\ell = 3$
  - m_ℓ = -3,-2,-1,0,+1,+2, +3 7 values

$\ell = 3$

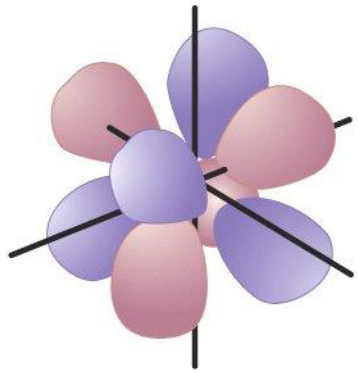
m_ℓ = -3,-2,-1,0,+1,+2, +3 7 values



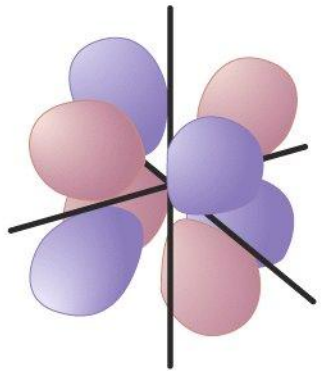
$5z^3 - 3zr^2$



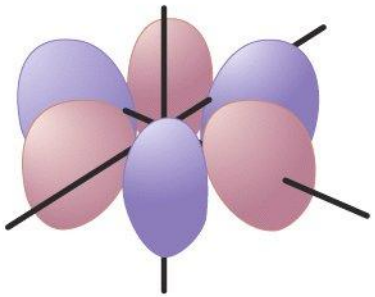
$5xz^2 - xr^2$



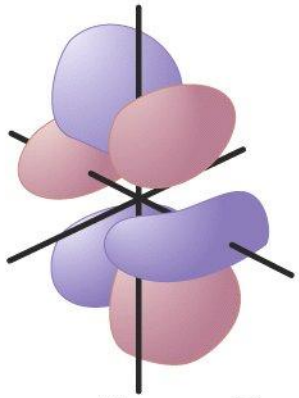
$zx^2 - zy^2$



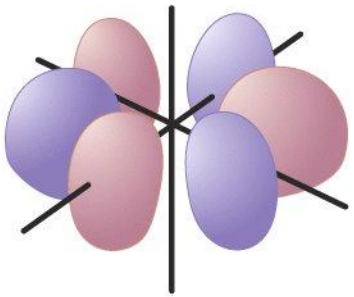
xyz



$y^3 - 3yx^2$



$5yz^2 - yr^2$



$x^3 - 3xy^2$

The fourth quantum number (s)

- **describes the spin of the electron + ½ or - ½**
- **If two electrons occupy the same space they have opposite spins**

Quantum Numbers

n – principal quantum number
l – orbital angular momentum
m_l – magnetic quantum number
m_s – spin quantum number

Hydrogen $1s^1$

Quantum Numbers

- PRINCIPAL: n energy level,

the distance the orbital is from the nucleus

(1, 2, 3, 4…)

- ANGULAR MOMENTUM: ℓ shape

(s = 0, p = 1, d = 2, f = 3)

- MAGNETIC: m_ℓ spatial orientation

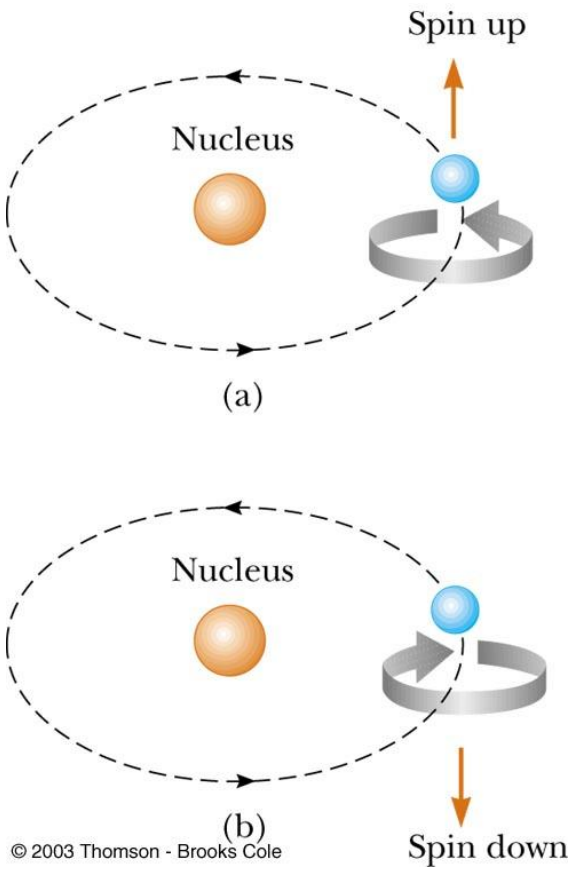
(0 for s; -1, 0, +1 for p; -2, -1, 0, +1, +2 for d, etc.)

- SPIN: m_s spin (+1/2 or -1/2)

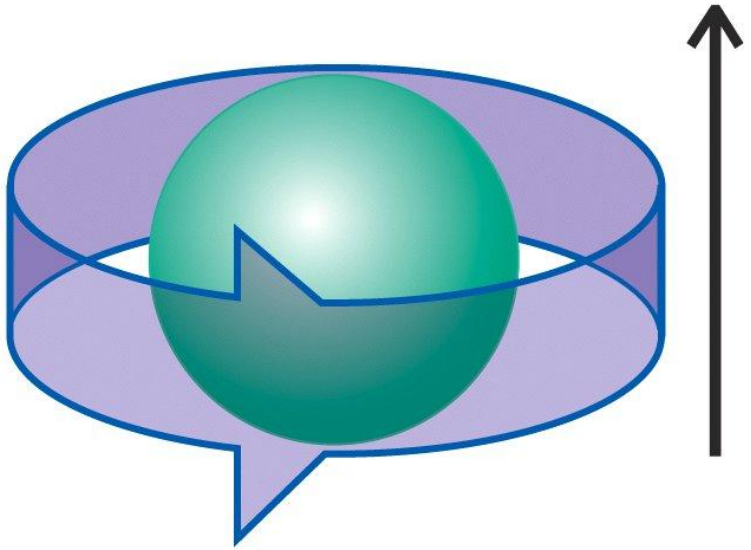
Spin quantum number

Spin Magnetic Quantum Number

- The last quantum number is the spin quantum number which has the symbol m_s.
- It is convenient to think of the electron as spinning on its axis
- There are two directions for the spin
- The spin quantum number only has two possible values.
  - $m_s = +1/2$ or $-1/2$
  - Spin up, $m_s = ½$
  - Spin down, $m_s = -½$
- There is a slight energy difference between the two spins and this accounts for the Zeeman effect

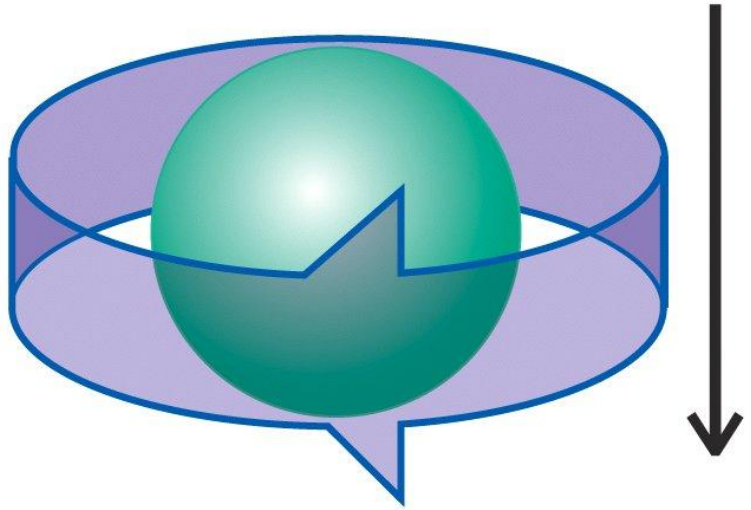


$m_s = +\frac{1}{2}$

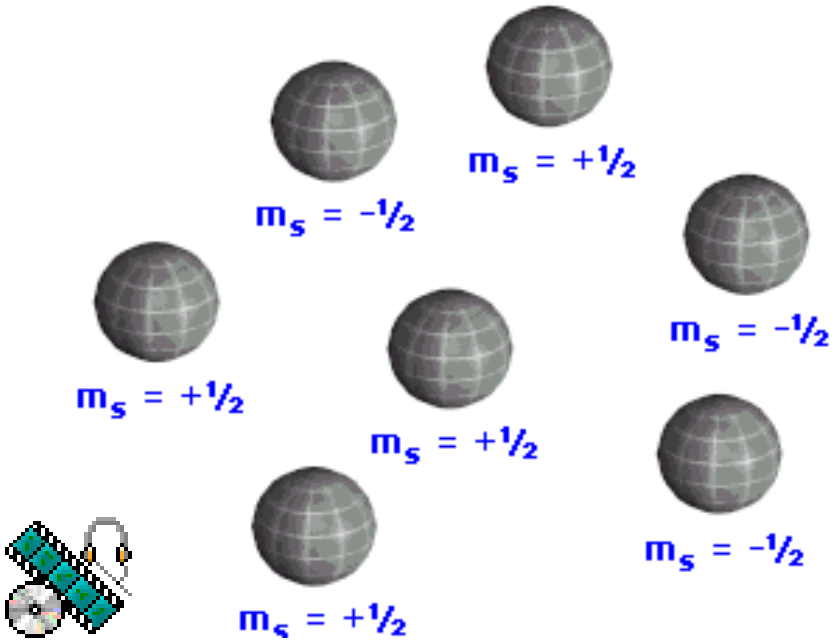


Spin of electron

$m_s = -\frac{1}{2}$



- Spin quantum number effects:
  - Every orbital can hold up to two electrons.
    - Consequence of the Pauli Exclusion Principle.
  - The two electrons are designated as having
  - one spin up ↑ and one spin down ↓
- Spin describes the direction of the electron's magnetic fields.



Re-Cap: Quantum Numbers

- PRINCIPAL: n energy level, distance from nucleus (1, 2, 3, 4…)

- ANGULAR MOMENTUM: ℓ shape
  (s = 0, p = 1, d = 2, f = 3)

- MAGNETIC: m_ℓ spatial orientation

(0 for s; -1, 0, +1 for p; -2, -1, 0, +1, +2 for d, etc.)

- SPIN: m_s spin (+1/2 or -1/2)

Quantum Number Summary

TABLE 28.2 **Three Quantum Numbers for the Hydrogen Atom**

Quantum Number	Name	Allowed Values	Number of Allowed States
n	Principal quantum number	$1, 2, 3, \ldots$	Any number
ℓ	Orbital quantum number	$0, 1, 2, \ldots, n-1$	n
m_ℓ	Orbital magnetic quantum number	$-\ell, -\ell+1, \ldots, 0, \ldots, \ell-1, \ell$	$2\ell+1$

- The values of n can increase from 1 in integer steps
- The values of ℓ can range from 0 to n-1 in integer steps
- The values of m_ℓ can range from $-\ell$ to ℓ in integer step

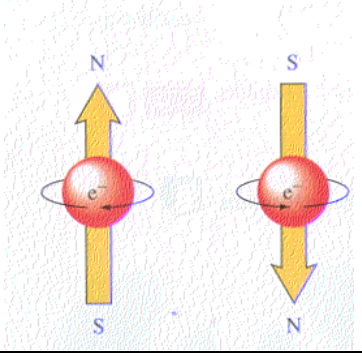
TABLE 1.3 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	$1, 2, \ldots$	shell	size
orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ $s, p, d, f, g, \ldots$	shape
magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

*Also called the *azimuthal quantum number.*

m_s = *spin magnetic* $\rightarrow$ electron spin

$m_s = \pm ½$ $(-½ = \alpha)$ $(+½ = \beta)$

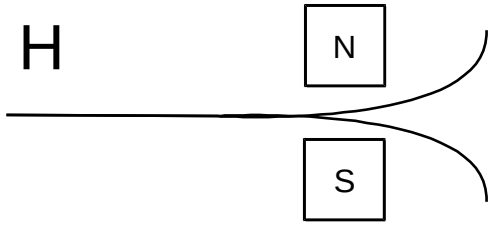


Pauli exclusion principle:

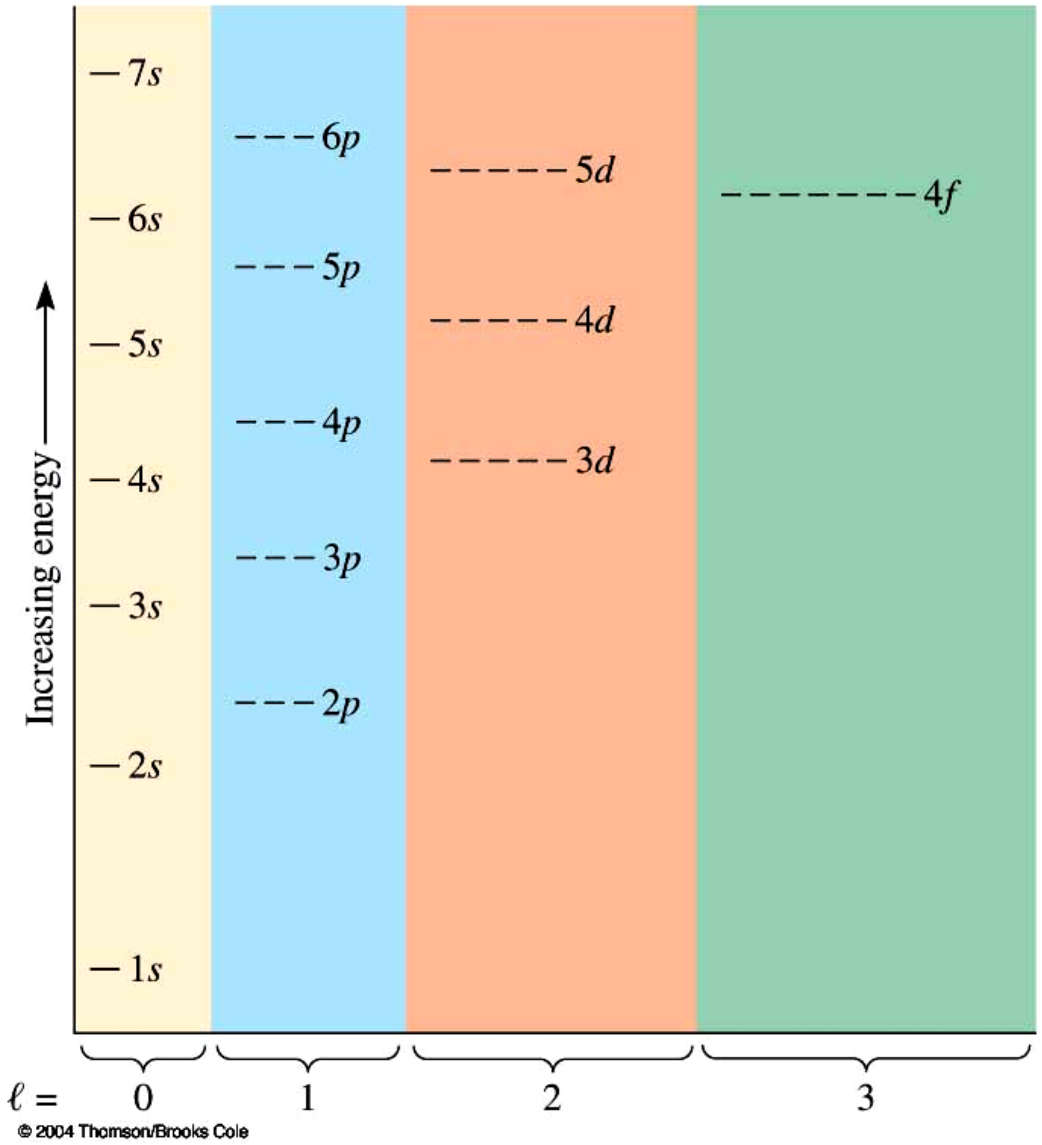
Each electron must have a unique set of quantum numbers.

Two electrons in the same orbital must have opposite spins.

Electron spin is a purely quantum mechanical concept.

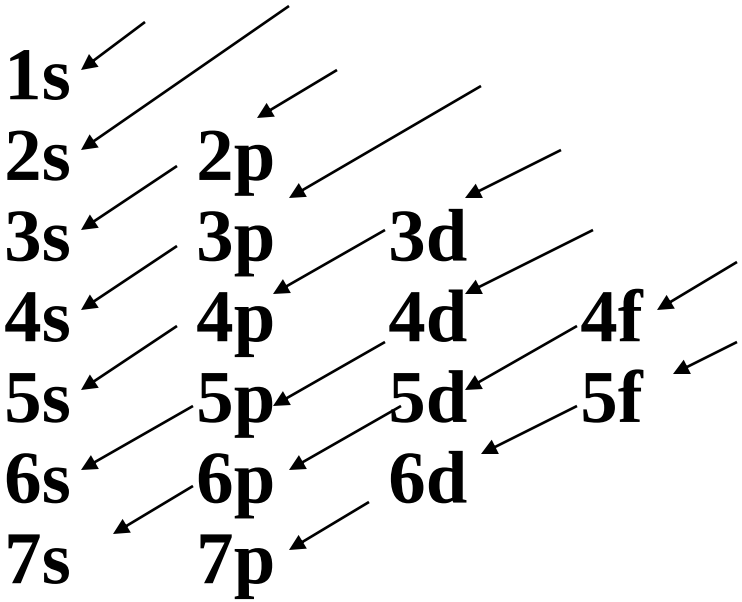


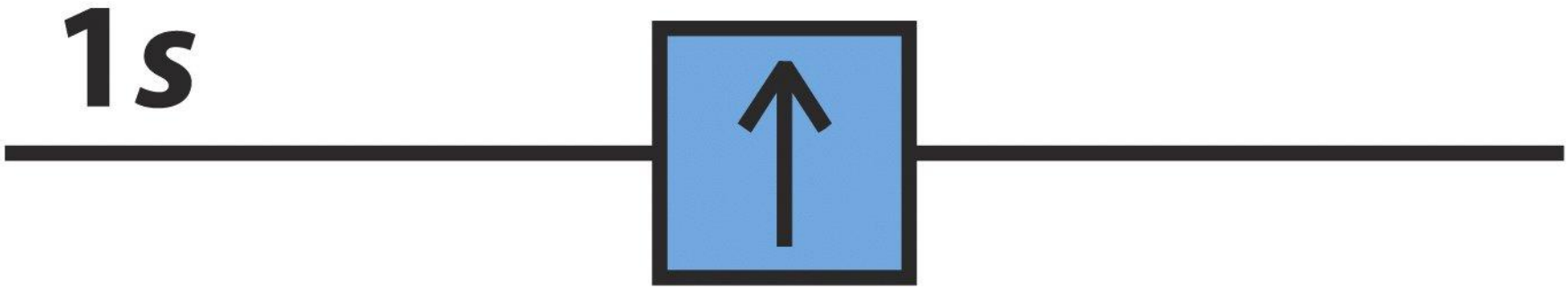
- The Aufbau Principle describes the electron filling order in atoms.



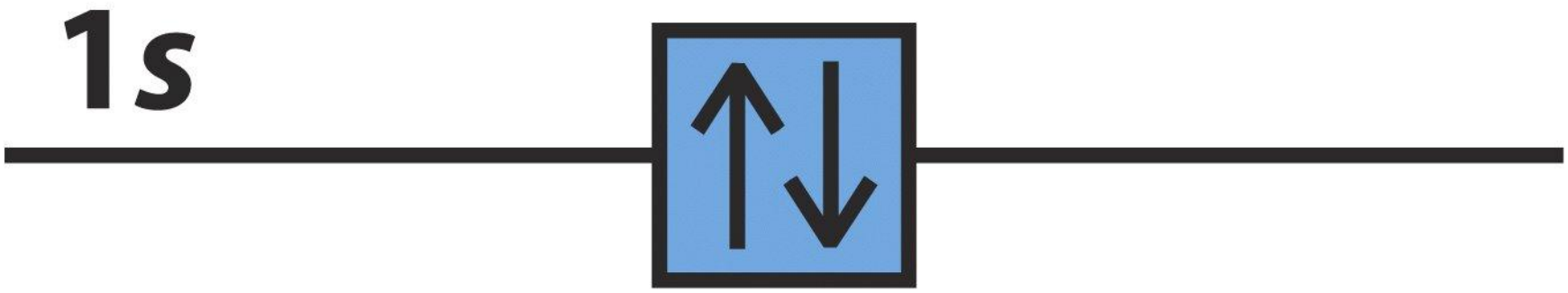
Diagonal rule

- **following the diagonals listing the orbitals you can find the electron configuration of most elements**

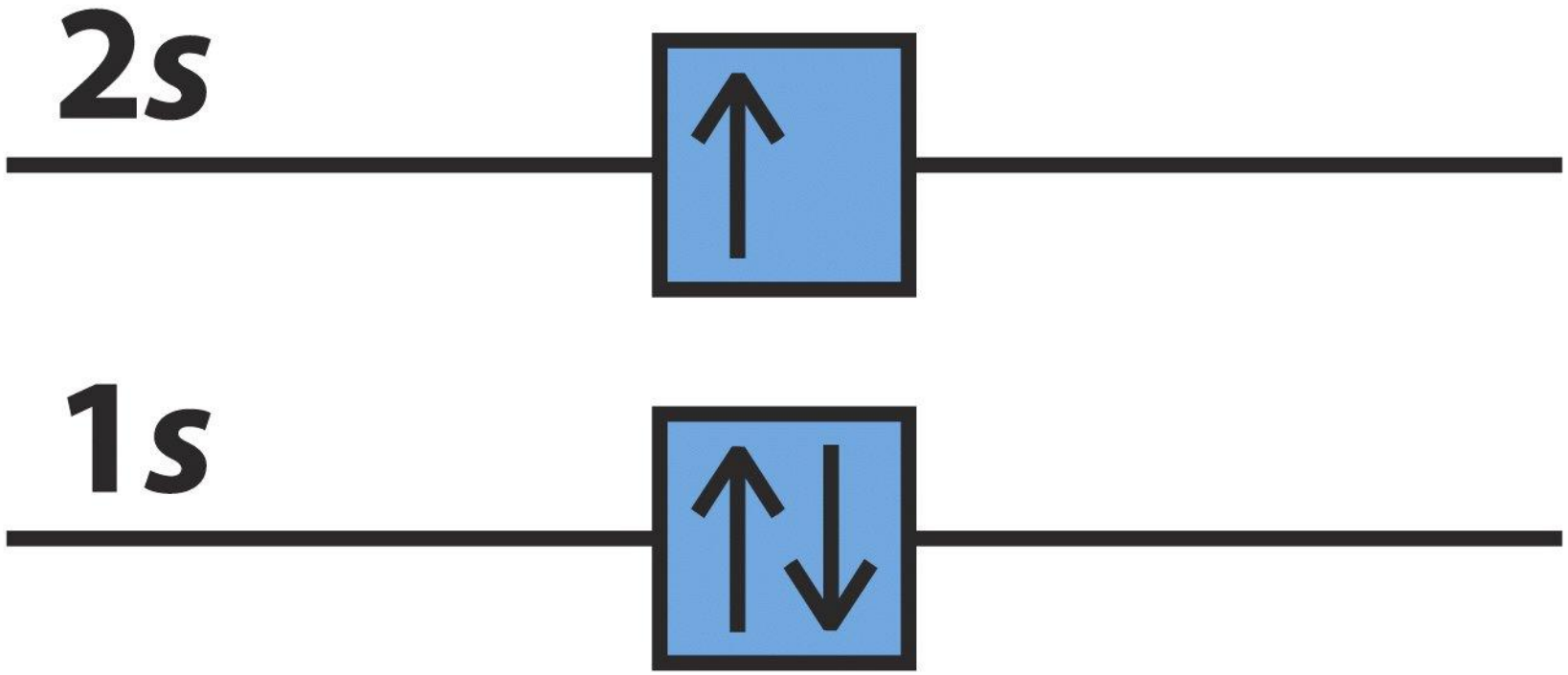




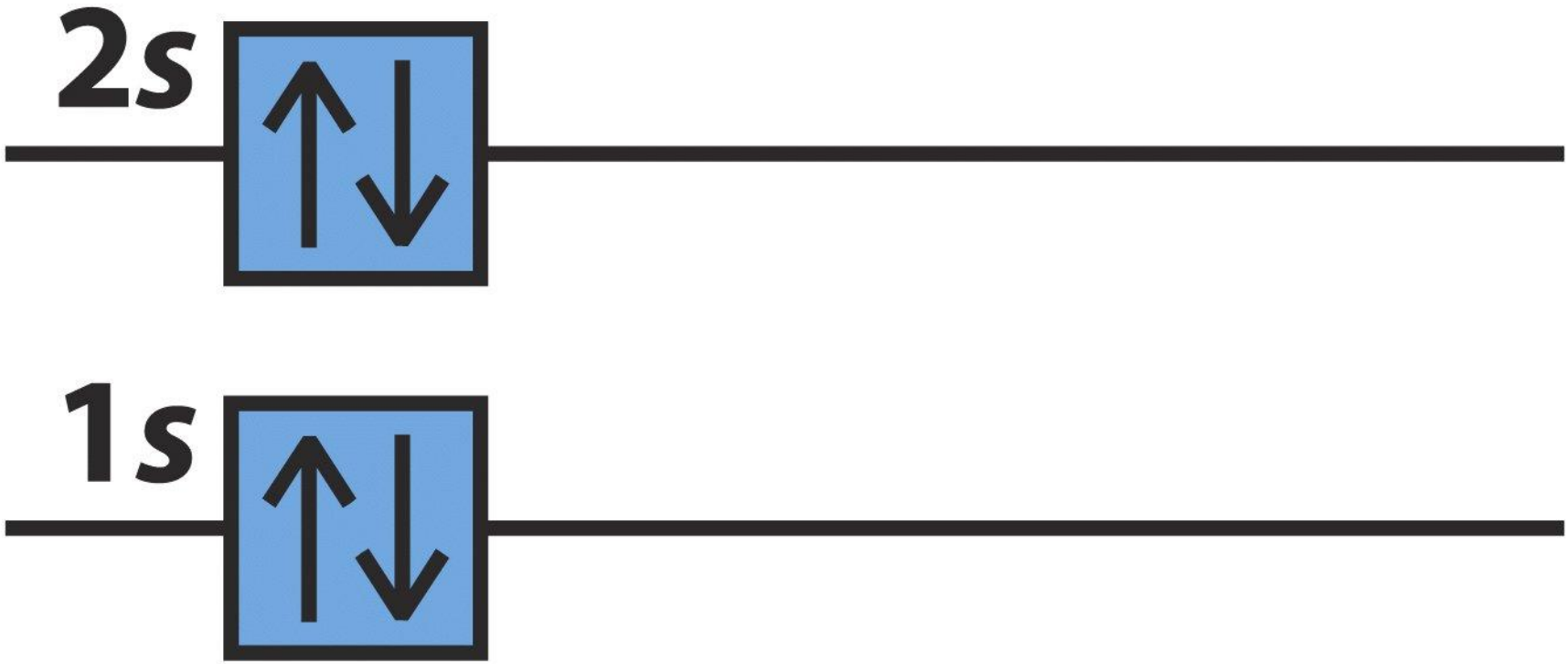
1 H $1s^1$



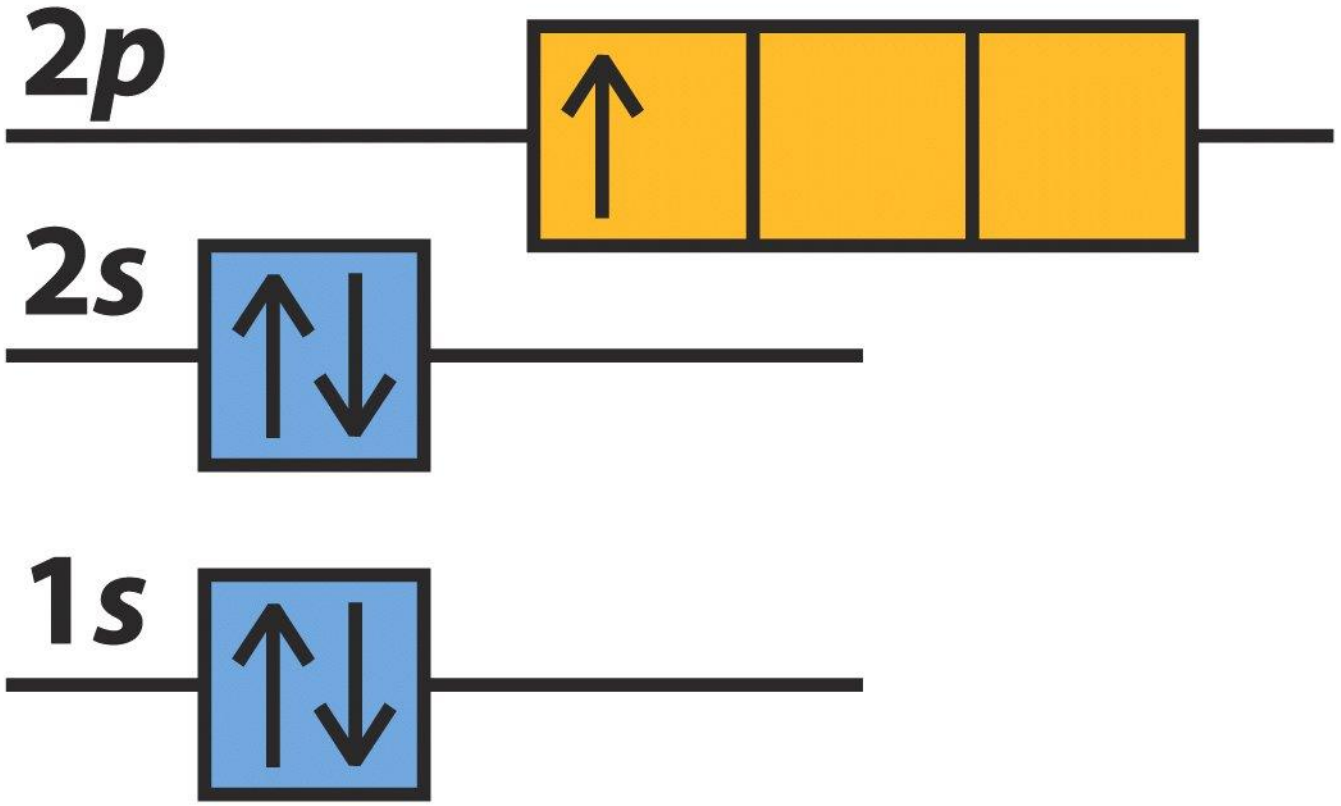
2 He $1s^2$



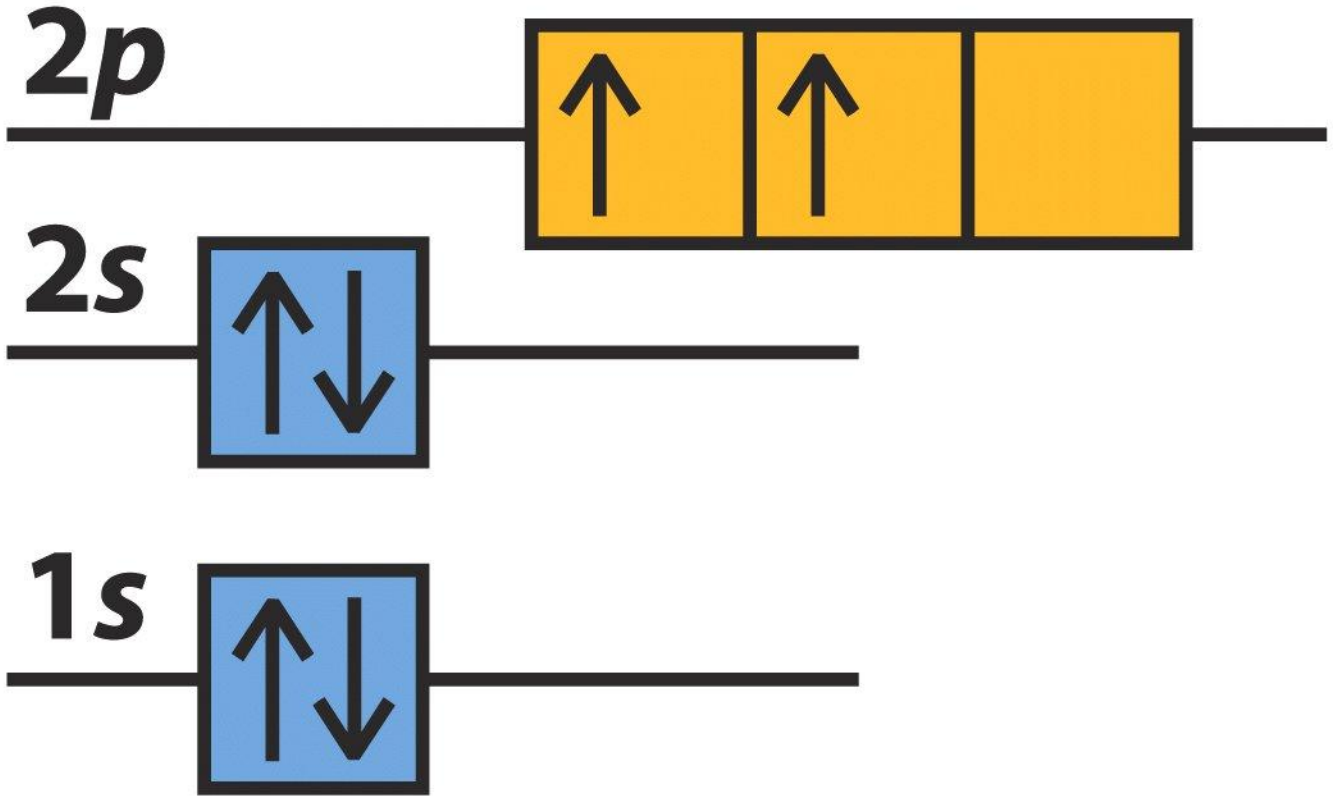
3 Li $1s^2 2s^1$, $[He]2s^1$



4 Be $1s^2 2s^2$, $[He]2s^2$



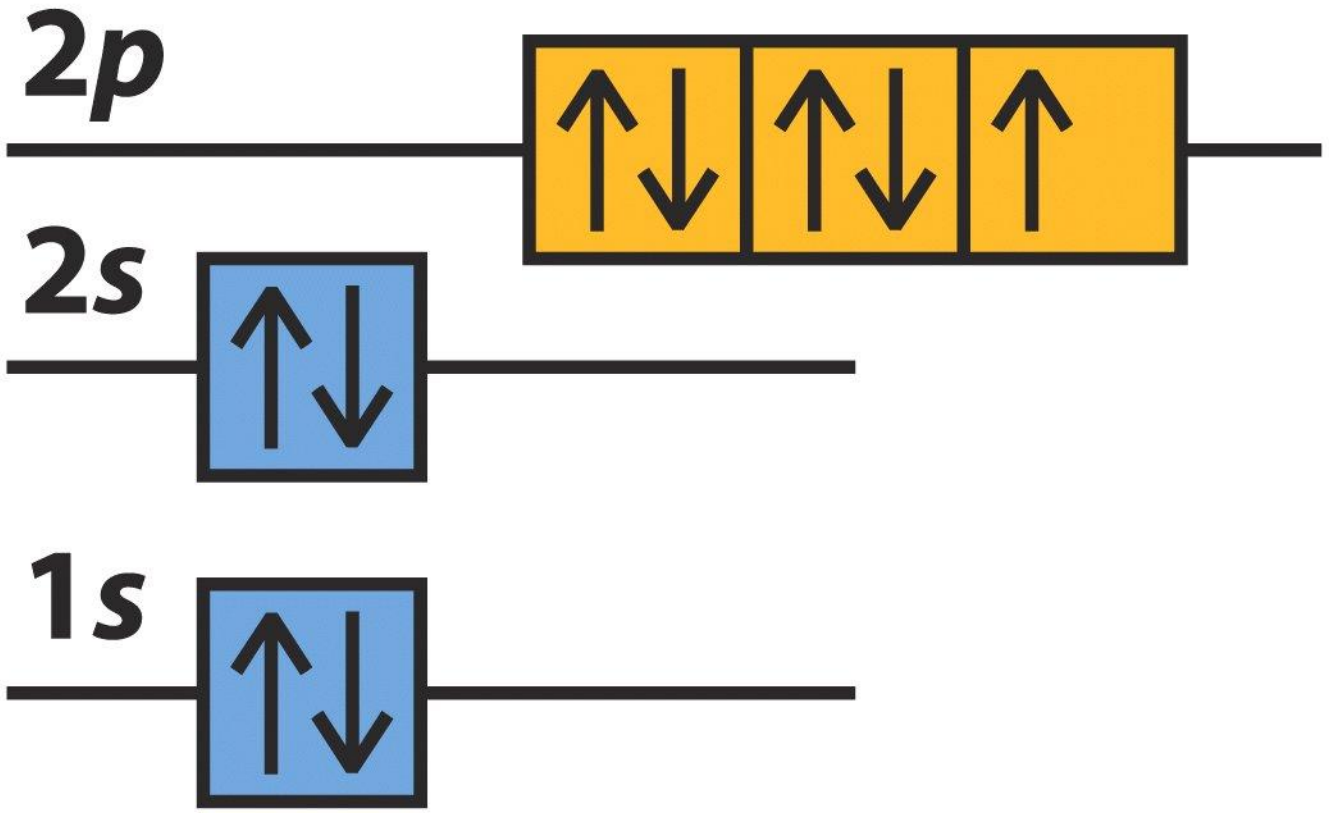
5 B $1s^2 2s^2 2p^1$, [He]$2s^2 2p^1$



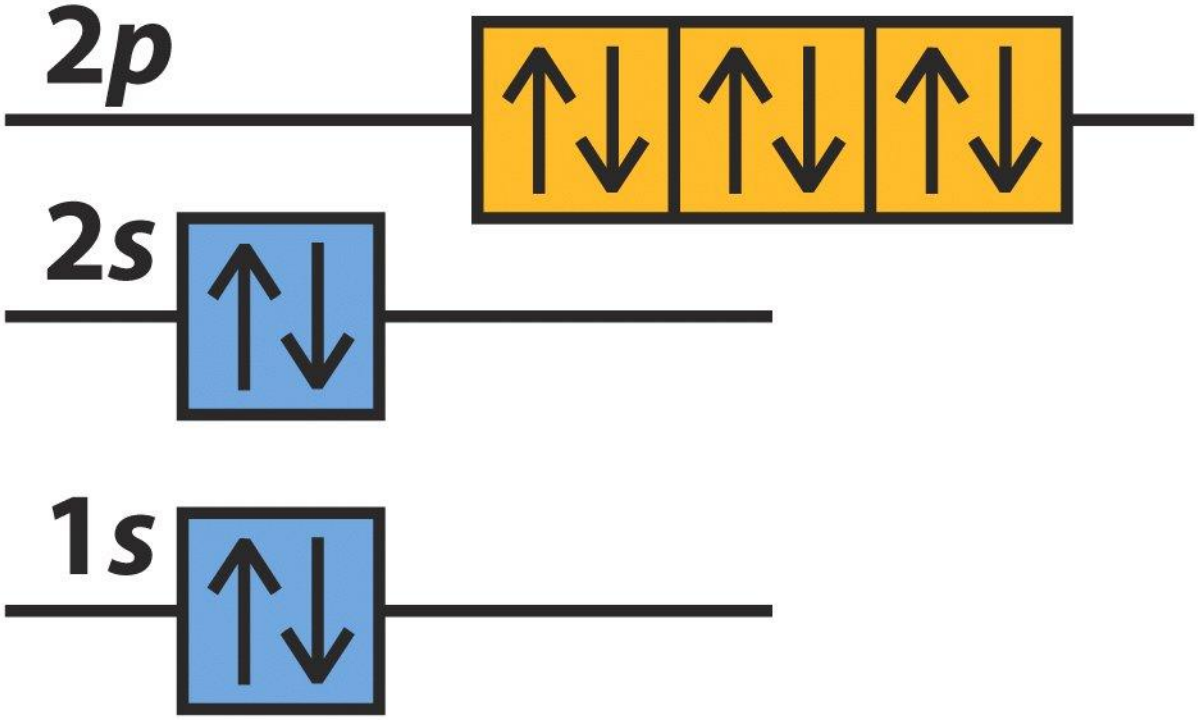
6 C $1s^2 2s^2 2p^2$, [He]$2s^2 2p^2$

•Hund's rule tells us that the electrons will fill the p orbitals by placing electrons in each orbital singly and with same spin until half-filled. Then the electrons will pair to finish the p orbitals.

	1s	2s	2p	Configuration
$_{3}$Li	↑↓	↑	_ _ _	$1s^2\ 2s^1$
$_{4}$Be	↑↓	↑↓	_ _ _	$1s^2\ 2s^2$
$_{5}$B	↑↓	↑↓	↑ _ _	$1s^2\ 2s^2\ 2p^1$
$_{6}$C	↑↓	↑↓	↑ ↑ _	$1s^2\ 2s^2\ 2p^2$
$_{7}$N	↑↓	↑↓	↑ ↑ ↑	$1s^2\ 2s^2\ 2p^3$
$_{8}$O	↑↓	↑↓	↑↓ ↑ ↑	$1s^2\ 2s^2\ 2p^4$
$_{9}$F	↑↓	↑↓	↑↓ ↑↓ ↑	$1s^2\ 2s^2\ 2p^5$
$_{10}$Ne	↑↓	↑↓	↑↓ ↑↓ ↑↓	$1s^2\ 2s^2\ 2p^6$

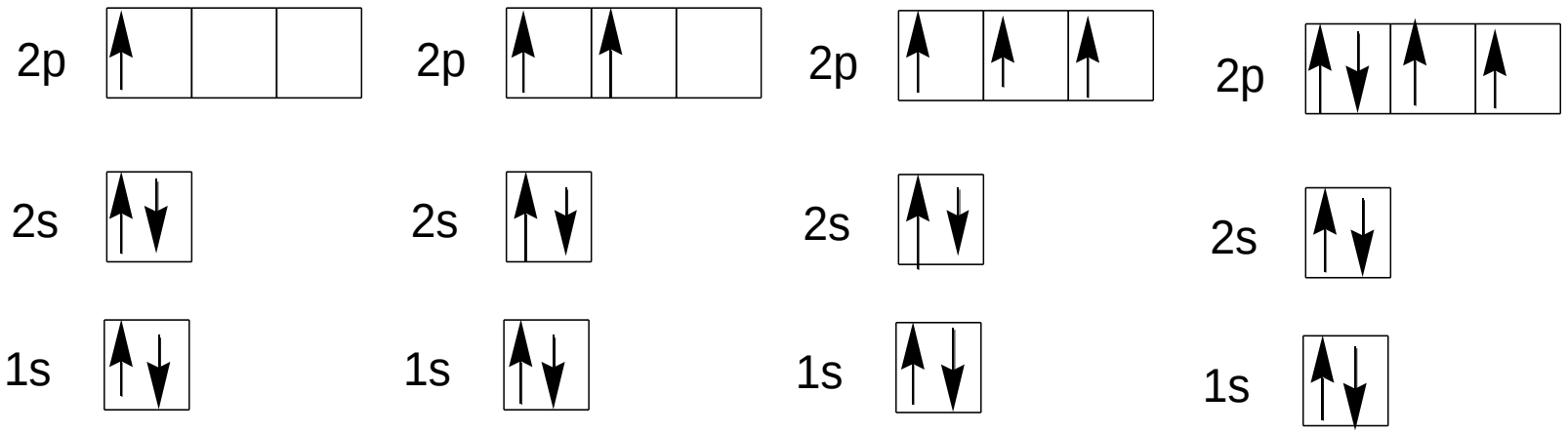


9 **F $1s^2 2s^2 2p^5$, [He]$2s^2 2p^5$**

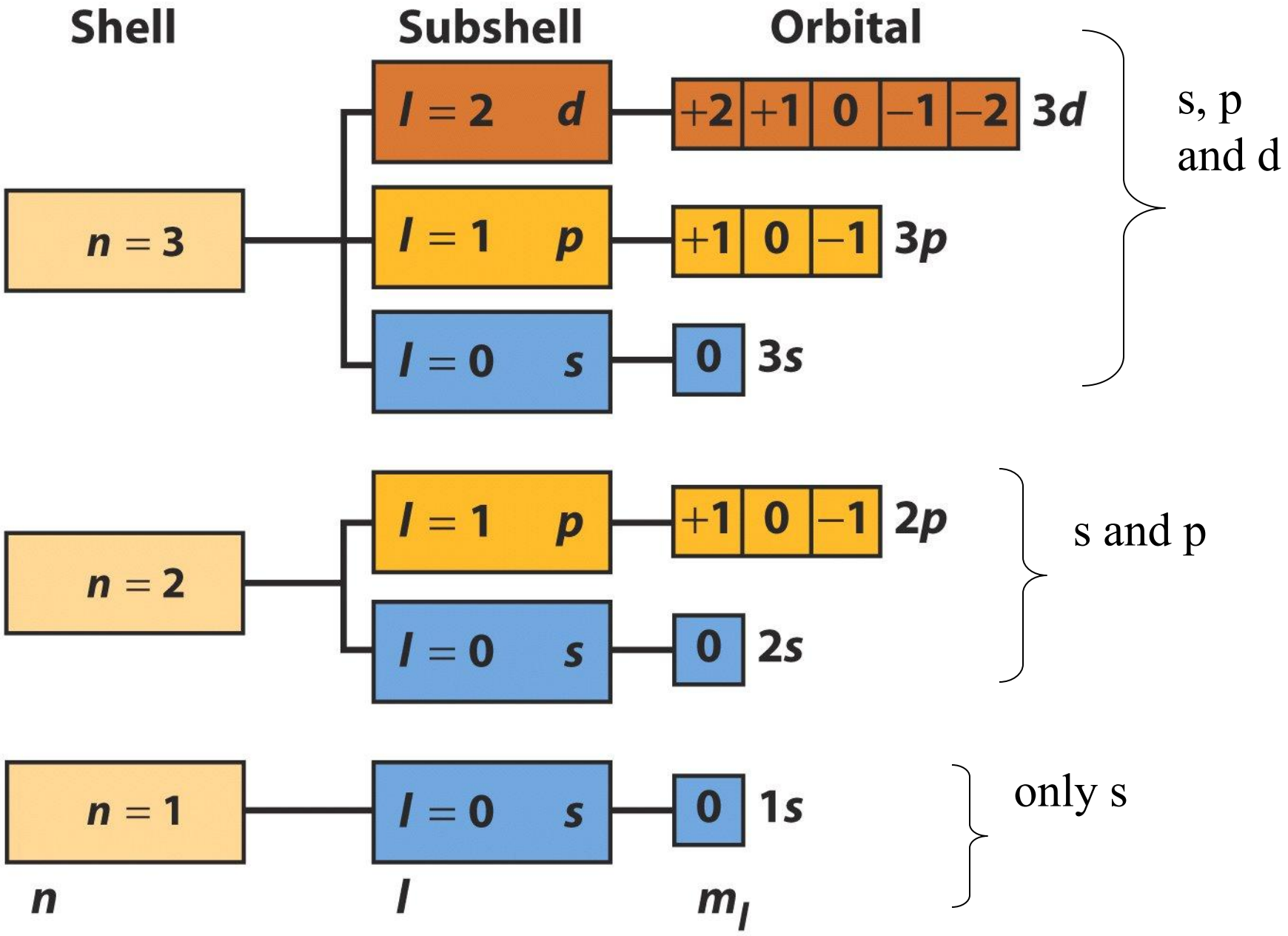


10 **Ne $1s^2 2s^2 2p^6$, [He]$2s^2 2p^6$**

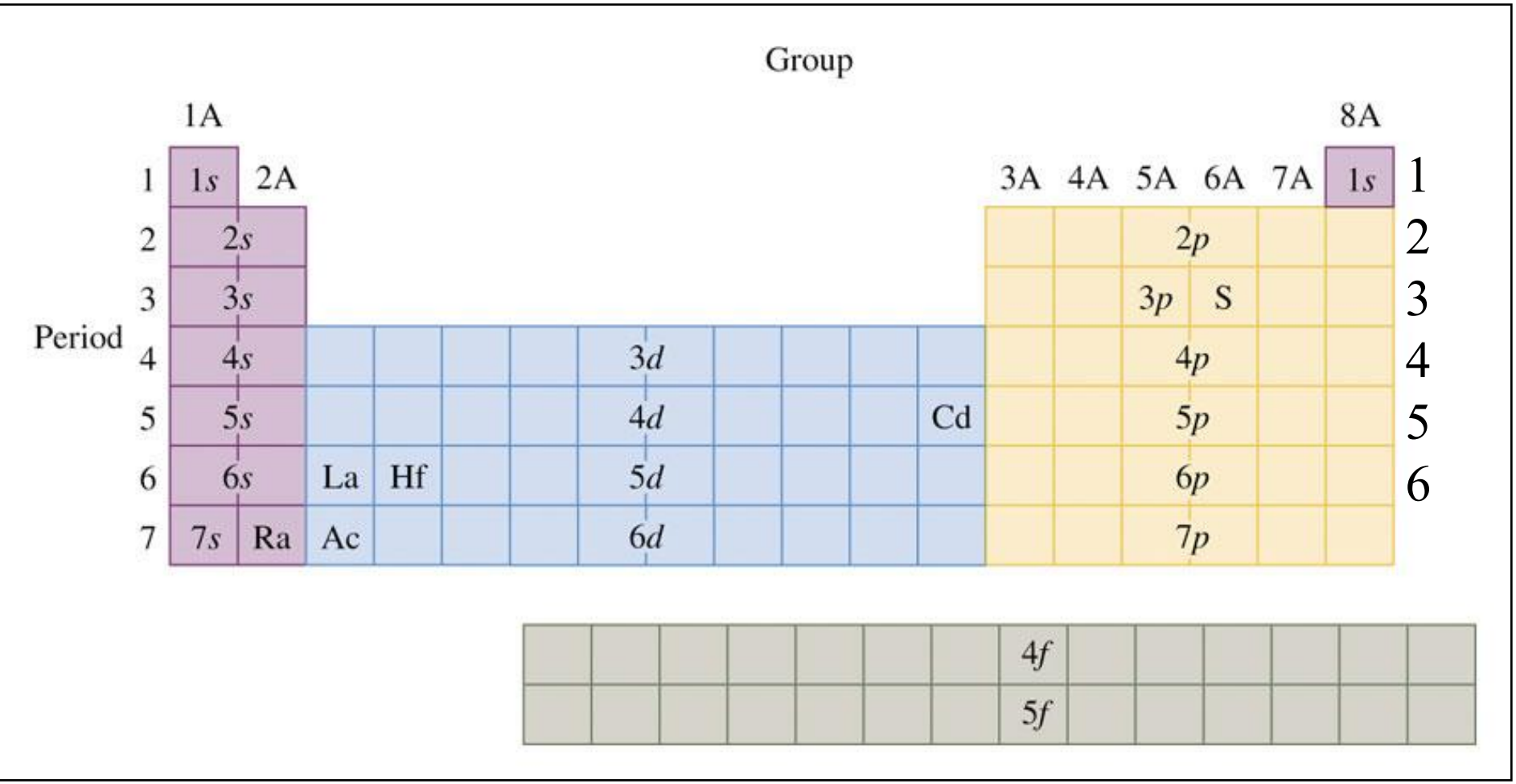
Electron Configurations



B	C	N	O
5	6	7	8


Shell
Subshell
Orbital
n = 3
l = 2 d
+2 +1 0 −1 −2
3d
l = 1 p
+1 0 −1
3p
l = 0 s
0
3s
s, p and d
n = 2
l = 1 p
+1 0 −1
2p
l = 0 s
0
2s
s and p
n = 1
l = 0 s
0
1s
only s
n
l
m_l

2. Or you can use the periodic chart .



- 3^{rd} row elements

		3s	3p	Configuration
$_{11}$Na	[Ne]	↑	_ _ _	[Ne]$3s^1$
$_{12}$Mg	[Ne]	↑↓	_ _ _	[Ne]$3s^2$
$_{13}$Al	[Ne]	↑↓	↑ _ _	[Ne]$3s^2\ 3p^1$
$_{14}$Si	[Ne]	↑↓	↑ ↑ _	[Ne]$3s^2\ 3p^2$
$_{15}$P	[Ne]	↑↓	↑ ↑ ↑	[Ne]$3s^2\ 3p^3$
$_{16}$S	[Ne]	↑↓	↑↓ ↑ ↑	[Ne]$3s^2\ 3p^4$
$_{17}$Cl	[Ne]	↑↓	↑↓ ↑↓ ↑	[Ne]$3s^2\ 3p^5$
$_{18}$Ar	[Ne]	↑↓	↑↓ ↑↓ ↑↓	[Ne]$3s^2\ 3p^6$

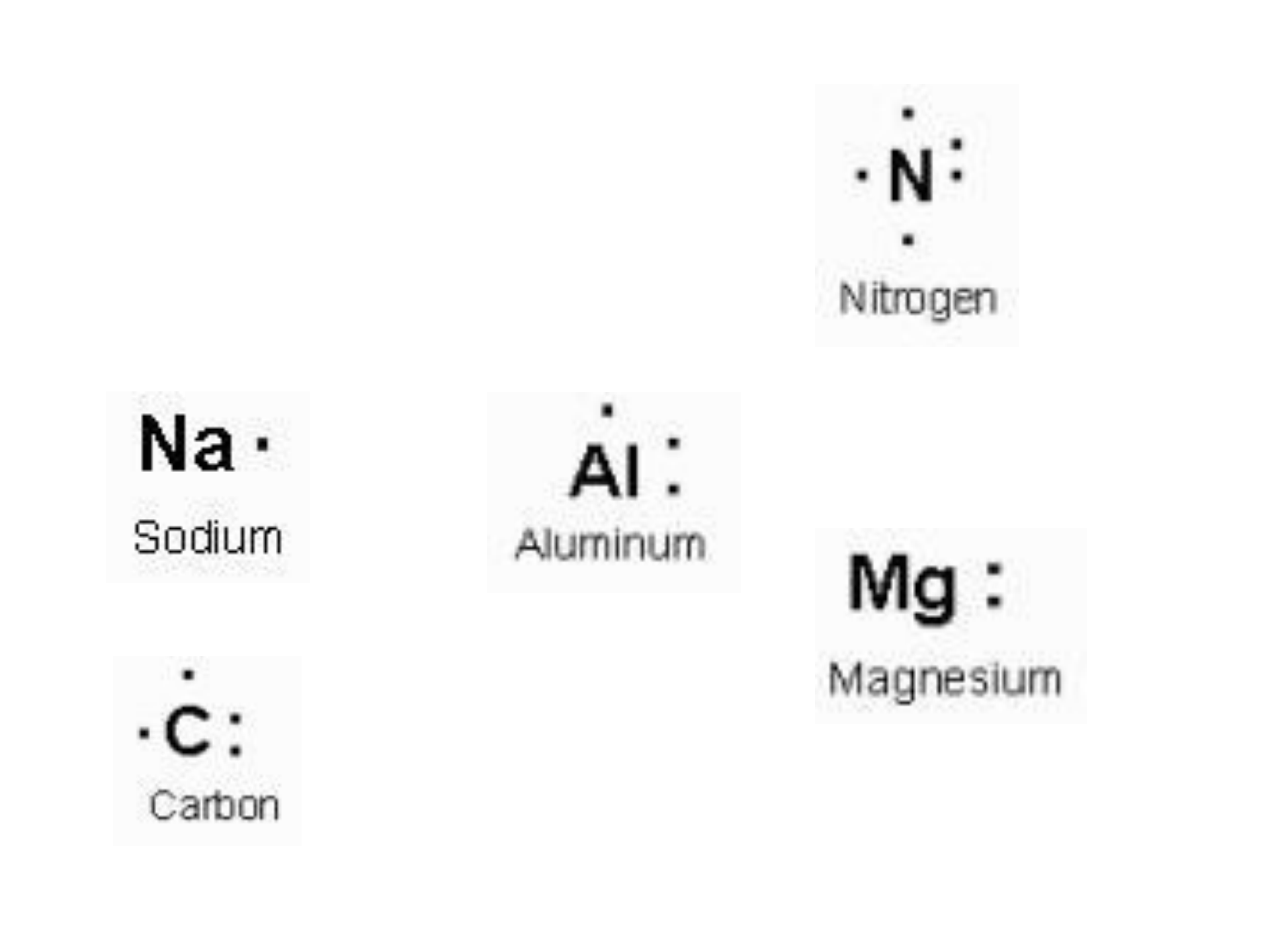
Fourth row

	3d	4s	4p	Configuration
$_{19}$K	[Ar] _ _ _ _ _	↑	_ _ _	[Ar] $4s^1$
$_{20}$Ca	[Ar] _ _ _ _ _	↑↓	_ _ _	[Ar] $4s^2$
$_{21}$Sc	[Ar] ↑ _ _ _ _	↑↓	_ _ _	[Ar] $4s^2$ $3d^1$
$_{22}$Ti	[Ar] ↑ ↑ _ _ _	↑↓	_ _ _	[Ar] $4s^2$ $3d^2$
$_{23}$V	[Ar] ↑ ↑ ↑ _ _	↑↓	_ _ _	[Ar] $4s^2$ $3d^3$
$_{24}$Cr	[Ar] ↑ ↑ ↑ ↑ ↑	↑	_ _ _	[Ar] $4s^1$ $3d^5$

There is an extra measure of stability associated with half - filled and completely filled orbitals.

Electron dot diagrams

- **Lewis Dot Diagram – a procedure used to show the outer electrons around the symbol**
  a. Let symbol represent the element's nucleus and all the electrons except the outer level
  b. Write the electron configuration for the element. From the configuration select the electrons from the highest principle quantum number
  c. Each "side" (top, bottom, left, right) of the symbol represents an orbital
  1) Draw dots on the appropriate sides to represent the electrons in the orbital
  2) Just the s and p orbitals are represented
  3) It is important which electrons are paired and which electrons are not paired


Nitrogen
Sodium
Aluminum
Magnesium
Carbon