

Atomic Structure & the periodic table

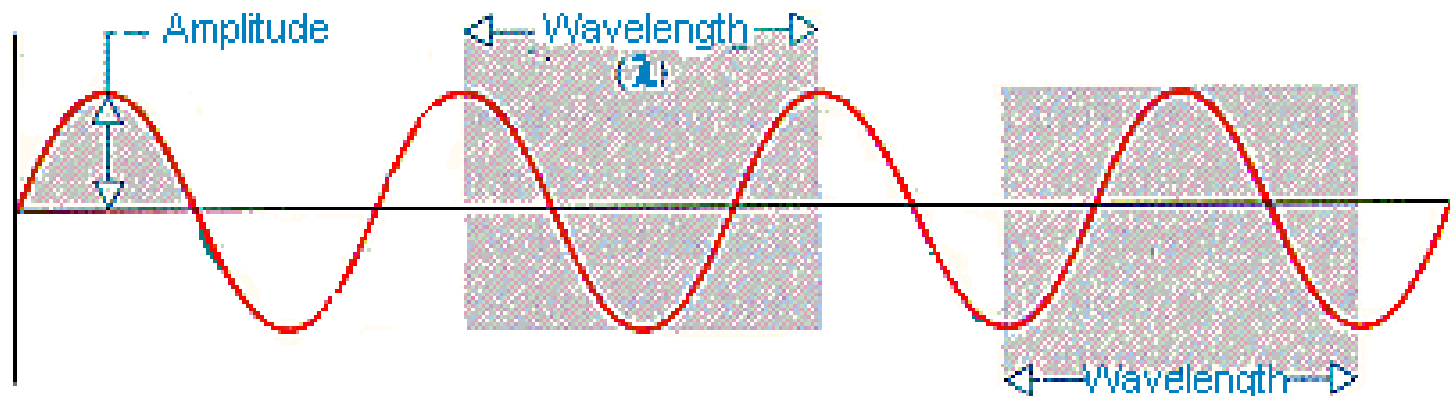
Electromagnetic Radiation

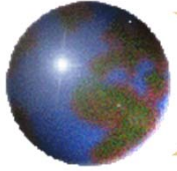
-travel through space in a wave motion

Terms used to describe waves

The wave length, λ (lambda):
the distance between two similar
Points on two successive waves.

The amplitude, a :
the height of a crest





**All waves travel at the same speed:
 2.9979×10^8 m/s {The speed of light (c)}**

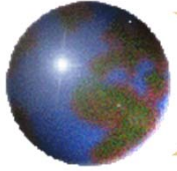
**The frequency, ν (nu): the number of waves that pass
A given spot in a second.**

$$\lambda \nu = c \Rightarrow \nu = \frac{c}{\lambda}$$

Example:

What is the frequency of the green traffic light ($\lambda = 522$ nm)

$$\nu = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m / s}}{522 \times 10^{-9} \text{ m}} = 5.75 \times 10^{14} \text{ s}^{-1} (\text{Hz})$$

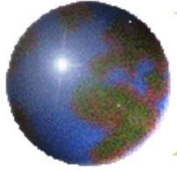


Example

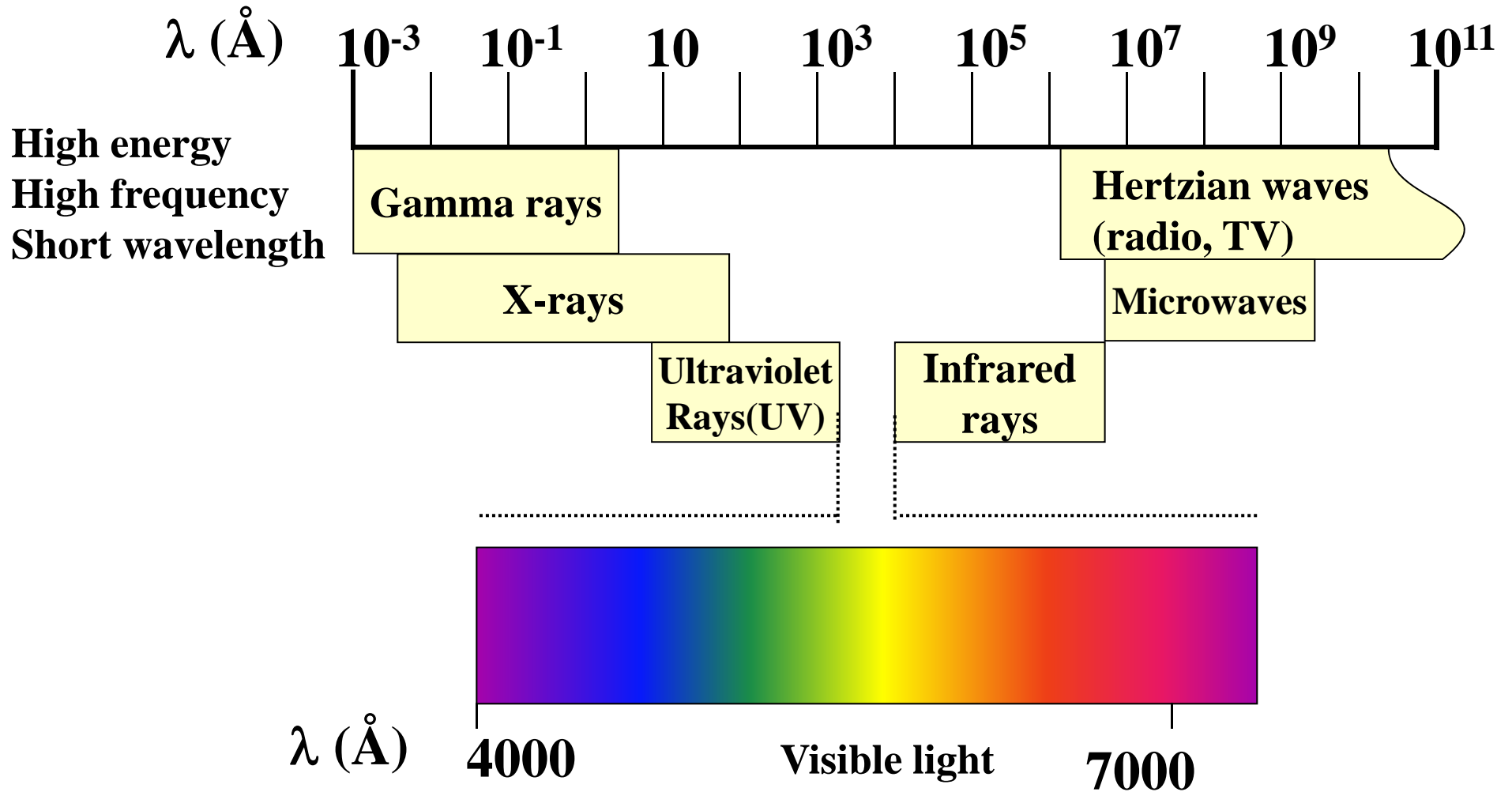
The frequency of the radio waves of a certain radiation is 106.5MHz.

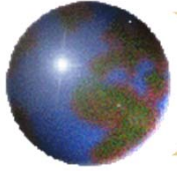
what is the wavelength of the waves in meters?

$$\nu = \frac{c}{\lambda} \Rightarrow \lambda = \frac{c}{\nu} = \frac{3.00 \times 10^8 \text{ m / s}}{106.5 \times 10^6 \text{ s}^{-1}} = 2.8 \text{ m}$$



The electromagnetic spectrum





In 1900, Max Planck proposed the quantum theory of radiant energy

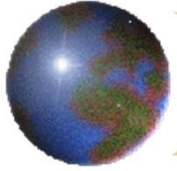
Radiant energy could be absorbed or given off only in definite quantities, called quanta

$$E = h \nu$$

E: energy of the quantum

ν : the frequency of the radiation

h: the proportionality constant, Planck's constant = 6.6262×10^{-34} J.s



Atomic spectra

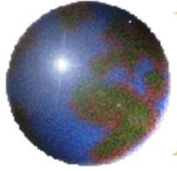
1913, *Niles Bohr*:

theory for the electronic structure of the hydrogen atom

The electron of the hydrogen atom can exist only in certain spherical orbits, also called energy levels or shells (K, L, M, N, O,.....)

The electron has an energy characteristic of the orbit in which it is moving

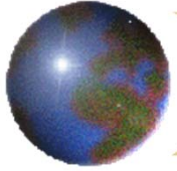
The K level ($n=1$) the shell closest to the nucleus, has the smallest radius, and the lowest energy



When the electrons of the atom are as close to the nucleus as possible they are in the condition of lowest possible Energy, called the *ground state*.

Electrons can absorb energy and jump to outer levels, which are higher energy levels.
In this case the atoms are said to be in *excited state*

When an electron falls back to a lower level, it emits a definite amount of energy.
The light quantum emitted has a characteristic frequency and produces a characteristic spectral line.



Bohr:

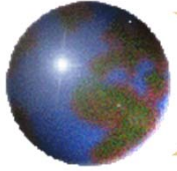
$$E_{orbit} = -\frac{2.179 \times 10^{-18} J}{n^2} \quad n = 1, 2, 3, \dots$$

$$h\nu = E_o - E_i \quad \text{for } E_o \rightarrow E_i$$

E_o = energy of the electron in an outer level

E_i = energy of the electron in an inner level

$$h\nu = \frac{-2.179 \times 10^{-18} J}{n_o^2} - \frac{-2.179 \times 10^{-18} J}{n_i^2}$$

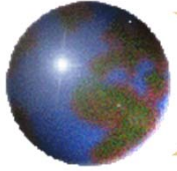


$$h\nu = 2.179 \times 10^{-18} \text{ J} \left(\frac{1}{n_i^2} - \frac{1}{n_o^2} \right)$$

$$h = 6.6262 \times 10^{-34} \text{ J}\cdot\text{s}$$

$$\nu = \frac{2.179 \times 10^{-18} \text{ J}}{6.626 \times 10^{-34} \text{ J}\cdot\text{s}} \left(\frac{1}{n_i^2} - \frac{1}{n_o^2} \right)$$

$$\nu = 3.289 \times 10^{15} \text{ s}^{-1} \left(\frac{1}{n_i^2} - \frac{1}{n_o^2} \right)$$

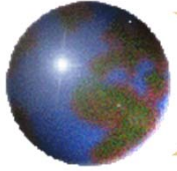


Example

Determine the frequency and the wavelength of the line in the hydrogen atom spectrum that results from the transition of an electron from the $n=3$ level to the $n=2$ level.

$$\nu = 3.289 \times 10^{15} \text{ s}^{-1} \left(\frac{1}{n_i^2} - \frac{1}{n_o^2} \right)$$

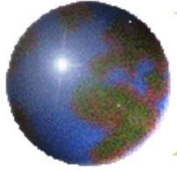
$$\nu = 3.289 \times 10^{15} \text{ s}^{-1} \left(\frac{1}{2^2} - \frac{1}{3^2} \right)$$



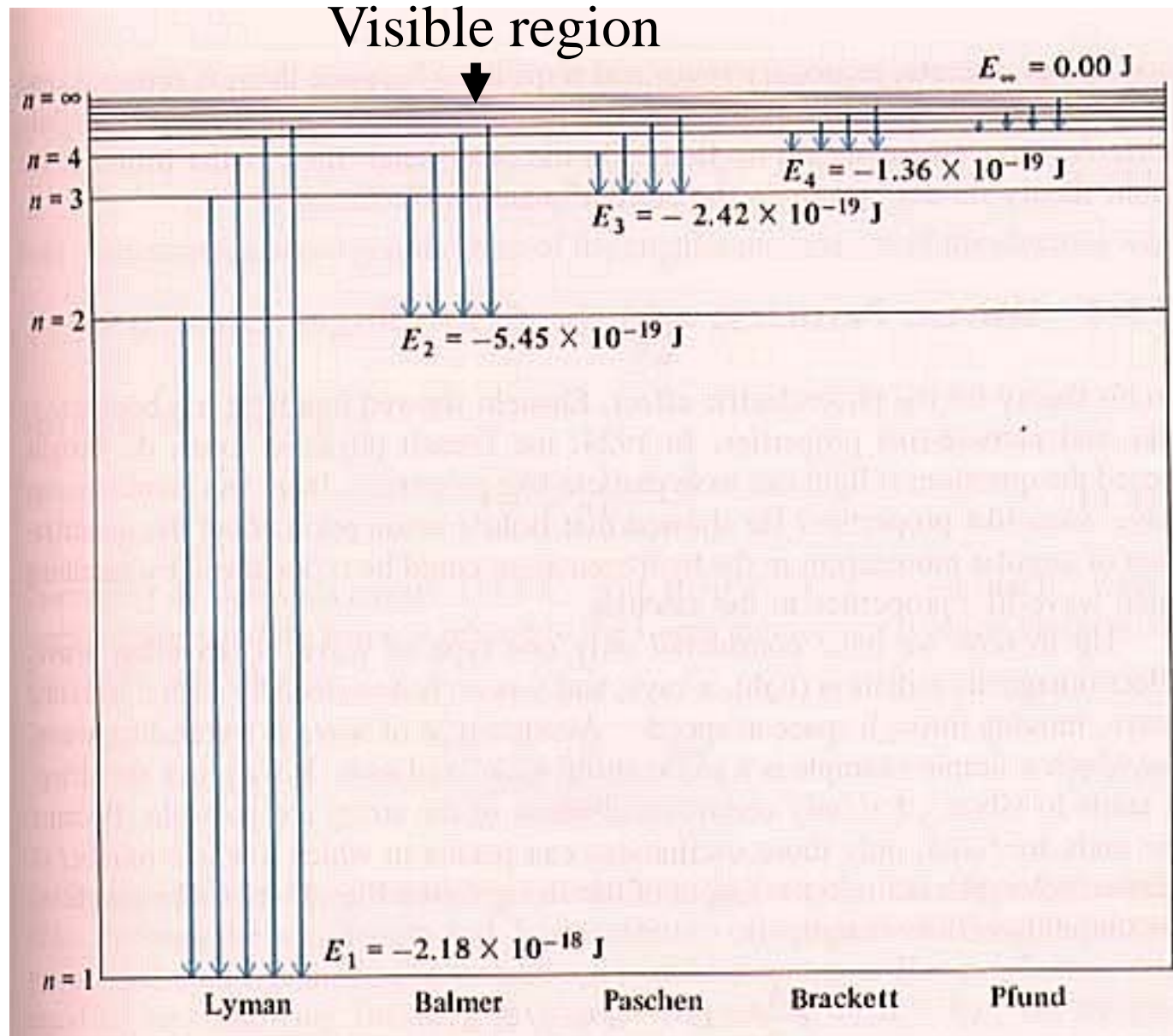
$$\nu = 3.289 \times 10^{15} \text{ s}^{-1} \left(\frac{1}{4} - \frac{1}{9} \right)$$

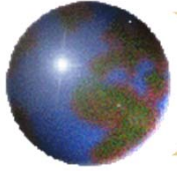
$$\nu = 4.568 \times 10^{14} \text{ s}^{-1} (\text{Hz})$$

$$\begin{aligned} \lambda &= \frac{c}{\nu} = \frac{3.0 \times 10^8 \text{ m/s}}{4.568 \times 10^{14} \text{ s}^{-1}} = 6.563 \times 10^{-7} \text{ m} \\ &= 656.3 \text{ nm} \end{aligned}$$



Hydrogen atom spectral series

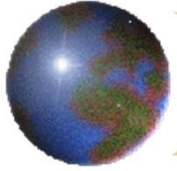




Bohr: the electron is a charged particle in motion, in the hydrogen atom it can only possess certain definite quantities of energy.

Werner Heisenberg, The uncertainty principle:
It is impossible to determine the exact position and exact momentum of the electron

Therefore, an exact description of the path of an electron in a *Bohr* orbit is not possible



1924, *Louis de Broglie*:

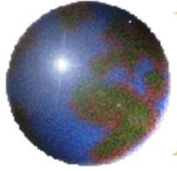
**Along with particle (mass) character, the electron
(and other particles) have wave properties**

$$\lambda = \frac{h}{mv}$$

h : Planck's constant

m : mass of the particle

v : velocity

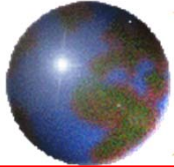


Example

Determine the de Broglie wavelength of an electron moving at 1.0% of the speed of light

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{9.11 \times 10^{-31} \text{ kg} \times 0.01 \times 3.00 \times 10^8 \text{ m/s}}$$
$$= 2.43 \times 10^{-10} \text{ m}$$

Remember: J = kg m² s⁻²



1926, *Erwin Schrödinger*, used the de Broglie relation to develop an equation that describes the electron in terms of its wave character, the Schrödinger equation is the basis of wave mechanics.

Quantum Numbers:

Each electron of an atom is identified by a combination of four quantum numbers

The principal quantum number, n :

Identifies the shell, or level to which the electron belongs

The larger the value of n , the farther the shell is from the nucleus.

$n = 1, 2, 3, \dots$



The angular momentum quantum number, l
Each shell consists of one or more subshell, or sublevel
 $l = 0, 1, 2, 3, \dots, (n-1)$

For $n = 1$

$l = 0$ only in the first shell we have only one subshell

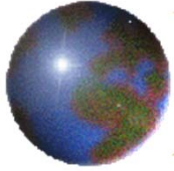
For $n = 2$

$l = 0, 1$ Here we have two subshells

Subshells are given notations,

$l = 0, 1, 2, 3, 4, \dots$

Notation = s, p, d, f, g, \dots



The magnetic quantum number, m_l

Each subshell consists of one or more orbitals, the number of orbitals in a subshell = $2l+1$

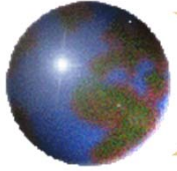
Each orbital is identified with m_l

$m_l = -l, -(l-1), \dots, 0, \dots, +(l-1), +l$

Magnetic spin quantum number, m_s

Can have only two values

$+1/2$ or $-1/2$



The four quantum numbers

1- n , gives the shell and the relative distance of the electron from the nucleus

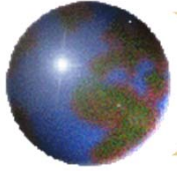
2- l , gives the subshell and the shape of the orbital for the electron

3- m_l , the orientation of the orbital

4- m_s , the spin of the electron



Shell(n)	Subshell(<i>l</i>)	Notation	Orbitals (m_l)
1	0	1s	0
2	0	2s	0
	1	2p	-1, 0, +1
3	0	3s	0
	1	3p	-1, 0, +1
	2	3d	-2, -1, 0, +1, +2
4	0	4s	0
	1	4p	-1, 0, +1
	2	4d	-2, -1, 0, +1, +2
	3	4f	-3, -2, -1, 0, +1, +2, +3



The exclusion principle (*Wolfgang Pauli*)

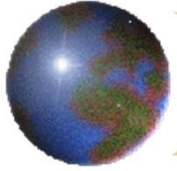
No two electrons in the same atom may have identical set of all four quantum numbers

This means:

1- an orbital may hold no more than two electrons.

2- if two electrons occupy an orbital they should have opposite spins

$$\text{i.e. } m_{s(1)} = +1/2 \text{ and } m_{s(2)} = -1/2$$



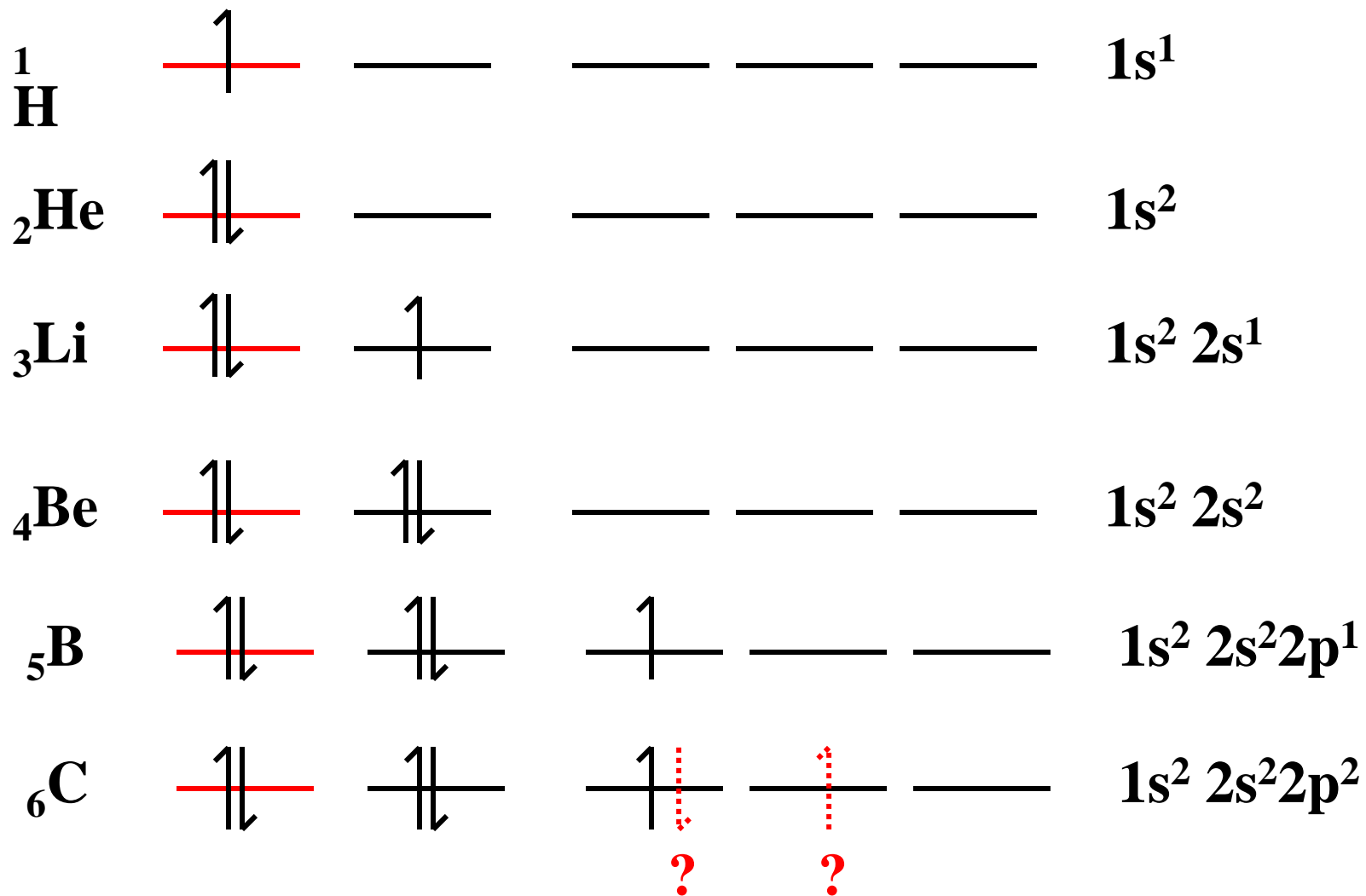
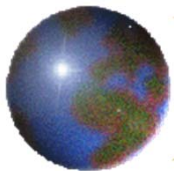
Electron configuration

Electron configuration:

The way electrons are arranged in an atom

For the first 18 elements the electron configuration can be assumed to result from electron occupying the shells by increasing value of n and l within the shell

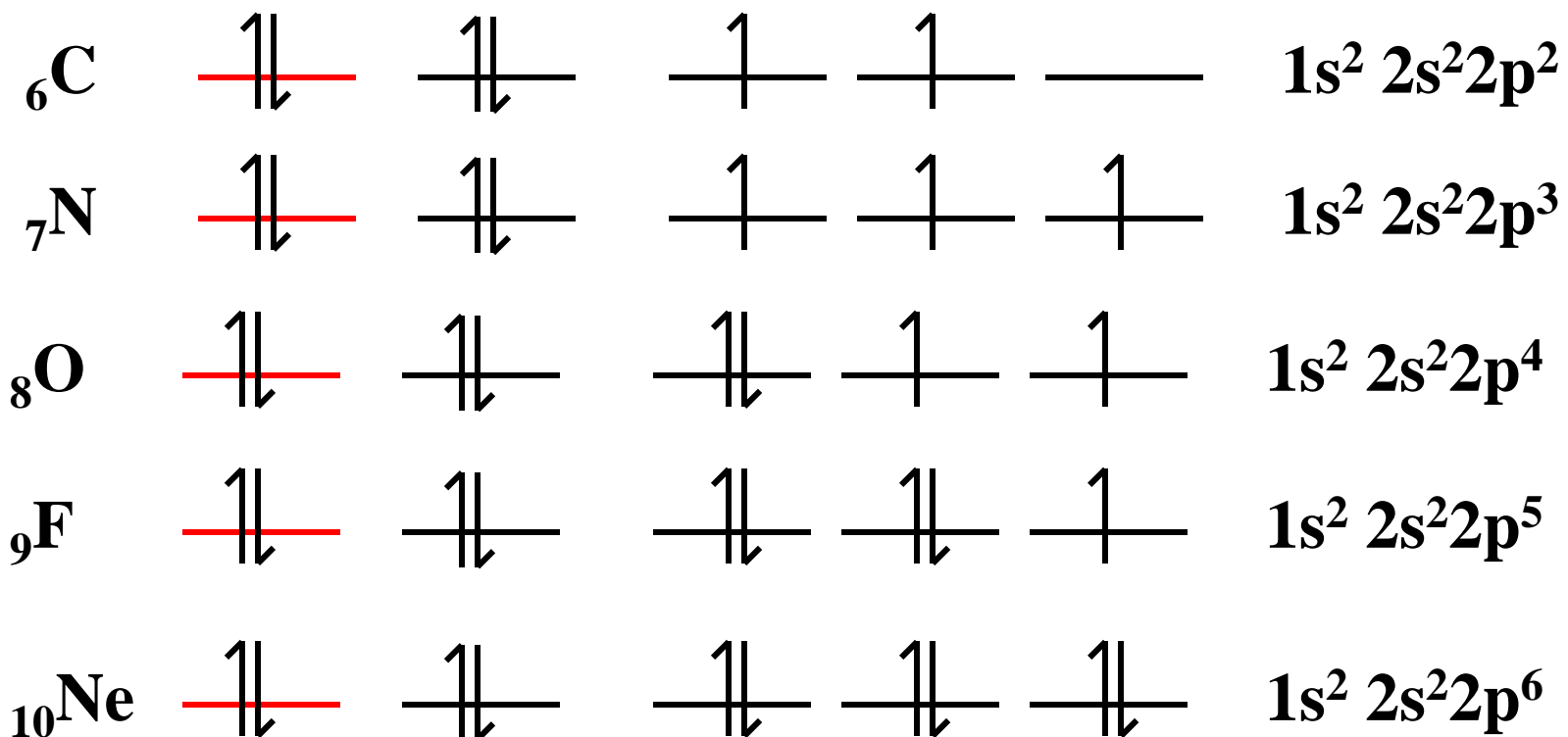
It gets complicated beyond $Z = 18$

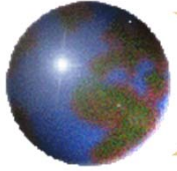




Hund's Rule

The most stable arrangement of electrons in a subshell is the one with the greatest number unpaired electrons with parallel spins





The number of unpaired electrons can be determined by magnetic measurements

Paramagnetic substances:

Are drawn into a magnetic field

Substances that contain unpaired electrons are

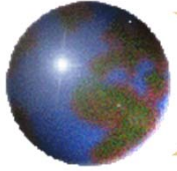
paramagnetic

Diamagnetic substances:

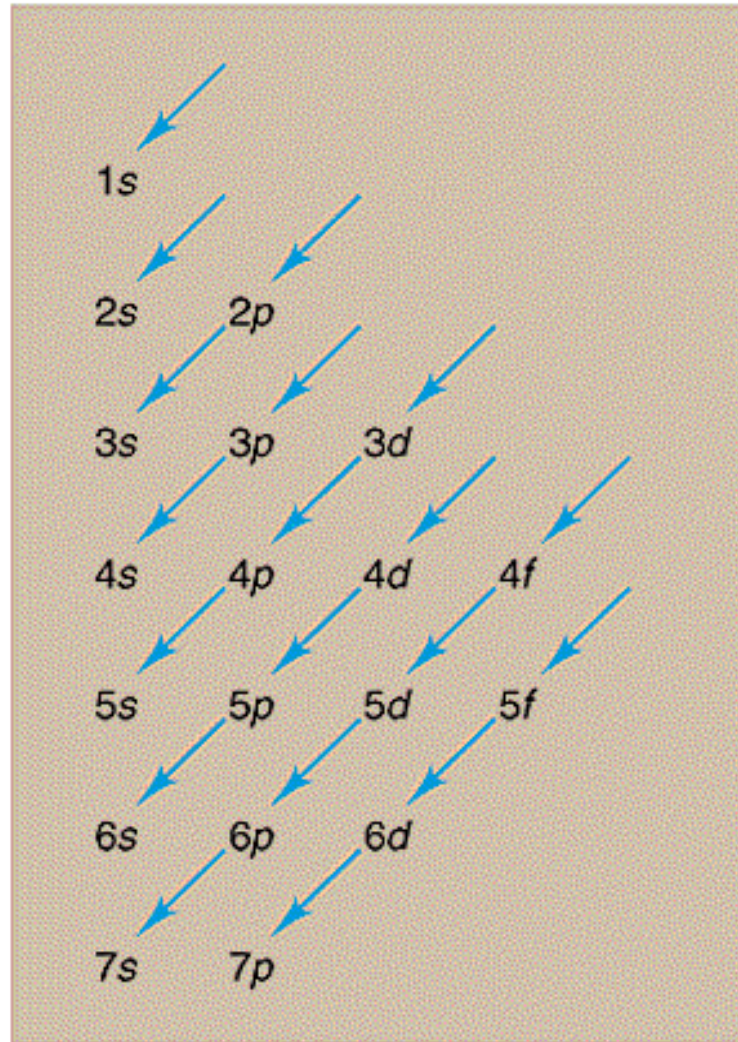
Are weakly repelled by a magnetic field

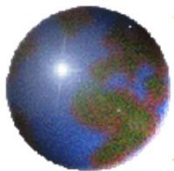
Substances in which all electrons are paired, are

diamagnetic



Aufbau method



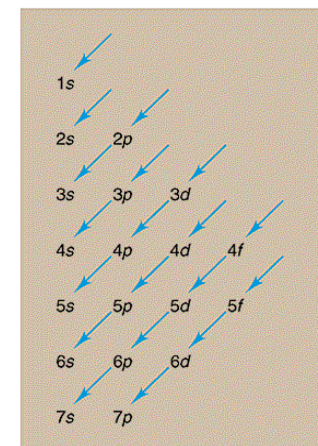
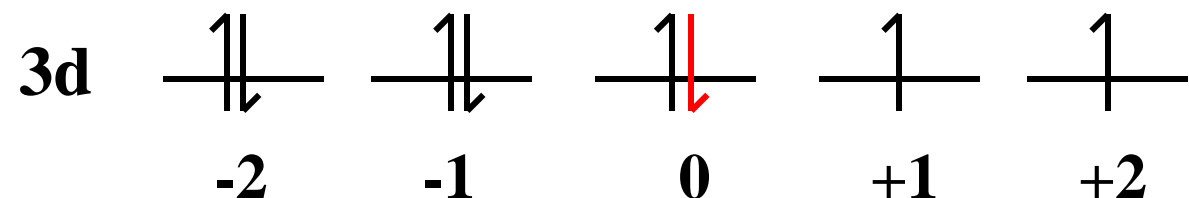
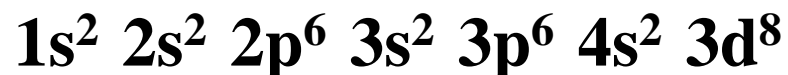


Example:

Write the electronic configuration of the $_{28}\text{Ni}$ atom.

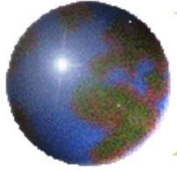
List the four quantum numbers of the differentiating electron

What is the magnetic property of the Ni atom?



$$n = 3 \quad l = 2 \quad m_l = 0 \quad m_s = -1/2$$

Magnetic property: Paramagnetic

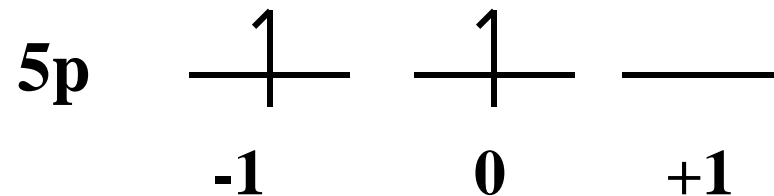
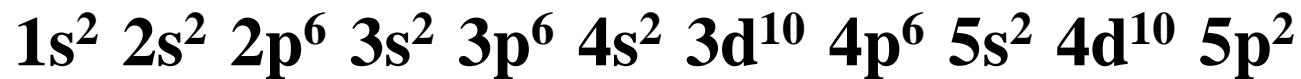


Example

Write the electronic configuration of the $_{50}\text{Sn}$ atom.

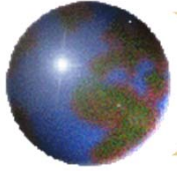
List the four quantum numbers of the differentiating electron

What is the magnetic property of the Sn atom?



$$n = 5 \quad l = 1 \quad m_l = 0 \quad m_s = +1/2$$

Magnetic property: paramagnetic

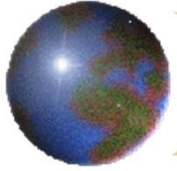


Exceptions to the aufbau method



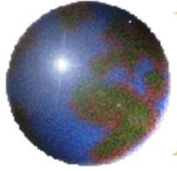
Explanation: stability is gained by having unpaired electron in each of the five 3d orbitals(half-filled)

${}_{42}\text{Mo}$: similar situation



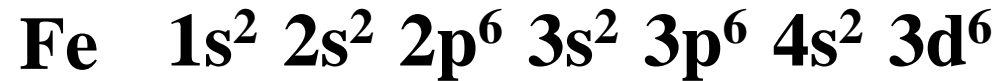
Explanation: stability is gained by having completely filled 3d subshell

${}_{47}\text{Ag}$ and ${}_{79}\text{Au}$: similar situation



Ionization

The aufbau method cannot be used to interpret ionizations



In general:

the first electrons lost in an ionization are those with the highest value of n and l