<u>Chemistry</u> = the study of matter: Properties
Structure
Transformations

STATES OF MATTER: Solid
(*ARRANGEMENT OF PARTICLES AND INTERACTIONS*) Liquid
Gaseous

PROPERTIES OF MATTER: PHYSICAL
<u>CHEMICAL</u>

STATE TRANSITIONS: PHYSICAL
REACTIONS (***compounds are formed***)

ENERGY: Kinetic (*Energy that can produce work*)
Potential (*Stored energy*)

<u>Chemical energy is a form of potential energy</u>

MATTER

ELEMENT: substance that can not be divided into other components by means of ordinary chemical reactions. (O, C, H, N, Au, Cu, Zn, Fe ...)

COMPOUND: consists of two or more elements combined in definite and constant proportions. A compound has properties different from those of its constituent elements.
(H_2O, $C_6H_{12}O_6$, HCl, NH_3 ...)

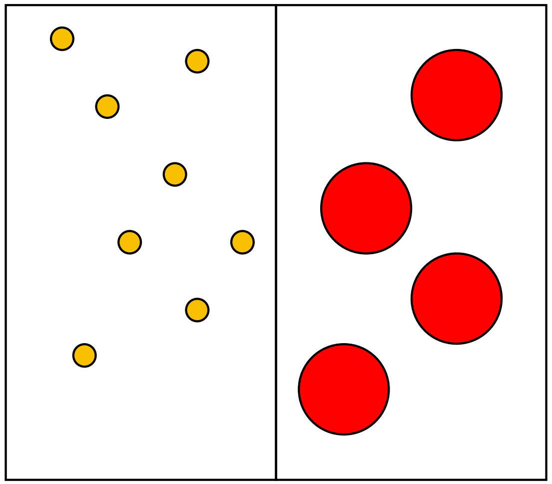
MIXTURES: consist of two or more substances combined in any proportion. The properties of the constituent elements remain unchanged.

HOMOGENEOUS MIXTURES: *Solution*

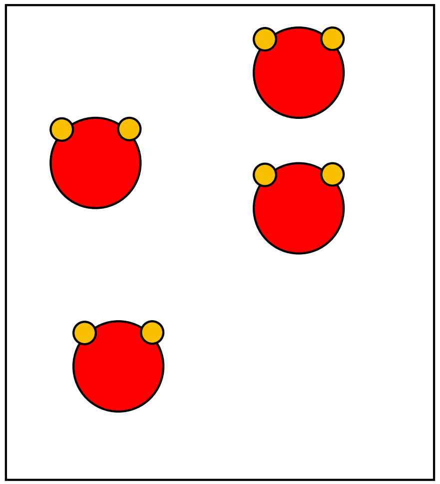
HETEROGENEOUS MIXTURES: suspension, mixture of solids

Atoms
element 1

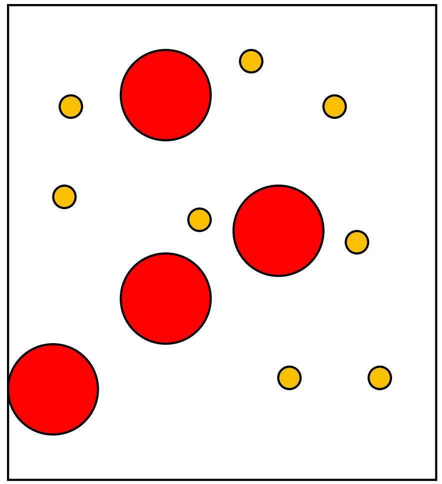
Atoms
element 2

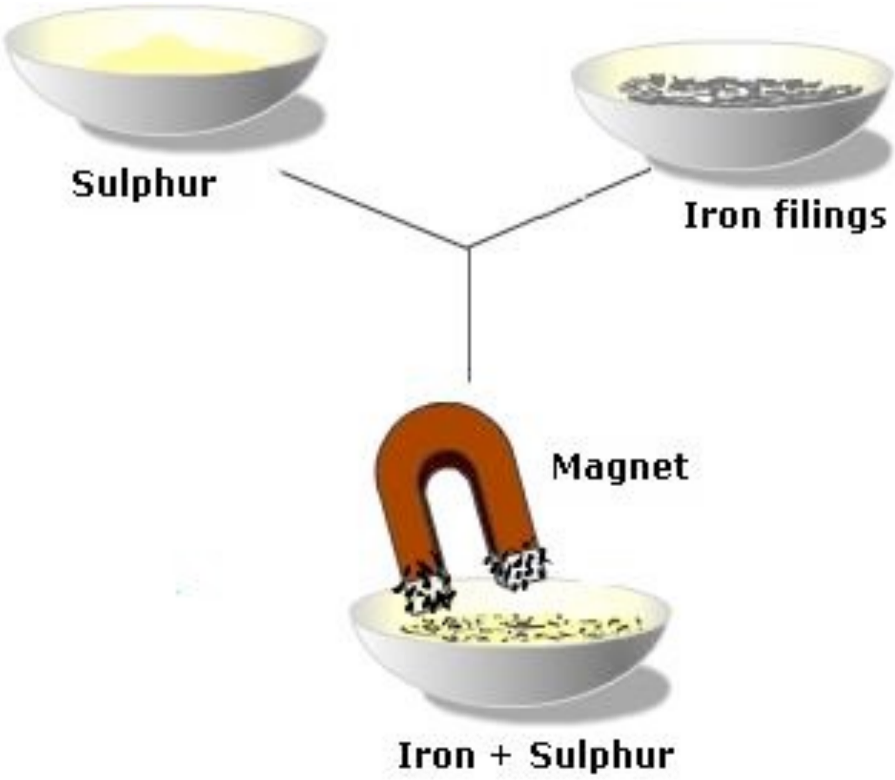


Compound formed by
elements 1 and 2



Mixture of
elements 1 and 2





Iron filings and sulphur

What physical difference between iron and sulphur could be used to separate them? Neither is soluble in water; they are both solids at room temperature; heating the mixture would cause them to react and produce iron sulphide. Iron is attracted to a magnet whereas sulphur is not, so you could use this difference to separate the two.

ELEMENTS FOUND IN LIVING MATTER

Carbon (C)
Hidrogen (H)
Nitrogen (N)
Oxygen (O)

The most abundant elements in living matter

Calcium (Ca)
Chloride (Cl)
Magnesium (Mg)
Phosphorus (P)
Potassium (K)
Sodium (Na)
Sulphur (S)
Elements present in small amounts and essential for life

Cobalt (Co)
Copper (Cu)
Iron (Fe)
Manganese (Mn)
Zinc (Zn)

Less abundant, but present in all organisms

Aluminum (Al)
Arsenic (Ar)
Boron (B)
Bromine (Br)
Chromo (Cr)
Fluoride (F)
Iodine (I)
Molybdenum (Mo)
Present in all organisms as trace elements.

Why do different types of atoms exist?

DALTON'S ATOMIC THEORY (1808):

- ✓ Every element is made up of particles called atoms.
- ✓ All atoms of a given element are identical.
- ✓ Atoms of different elements have different properties (eg. mass).
- ✓ Chemical reactions do not change atoms of one element into those of another; (in chemical reactions the atoms are neither created nor destroyed)
- ✓ Compounds are given by the combination of at least two elements.
- ✓ In a given compound the relative amount of atoms and their type are constant.

The atom is the smallest poortion of an element that maintains its characteristics

What is the difference between atoms in differenet elements?

THE STRUCTURE OF THE ATOMS

ATOM: indivisible unit composed of a central core surrounded by electrons

- NUCLEUS: protons, endowed with a positive charge (+)
  +
  neutrons, not charged

- ELECTRONS

Protons and neutrons have the same mass ($1{,}6 \times 10^{-24}$g), the mass of an electron is 1/1800 of the the mass of a proton.
The atomic radius is about 1 Å (10^{-10} m). The radius of the nucleus is about 10^{-15} m.

•If the nucleus had a radius = 1 cm,
The atomic radius would be equal to 1 km.

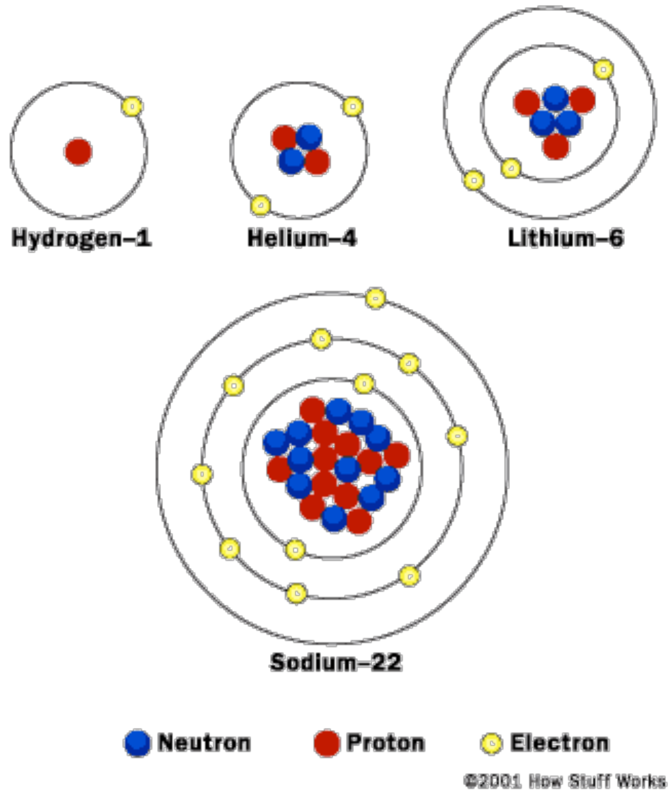
Atoms differ from each other in the number of elementary particles (protons, neutrons, electrons) that compose them.
We distinguish the different elements using unique names and symbols.

Z = atomic number = n° di protons in the nucleus
A = mass number = n° protons + n° neutrons

A =p+n

$^{1}_{1}H$

Z=p



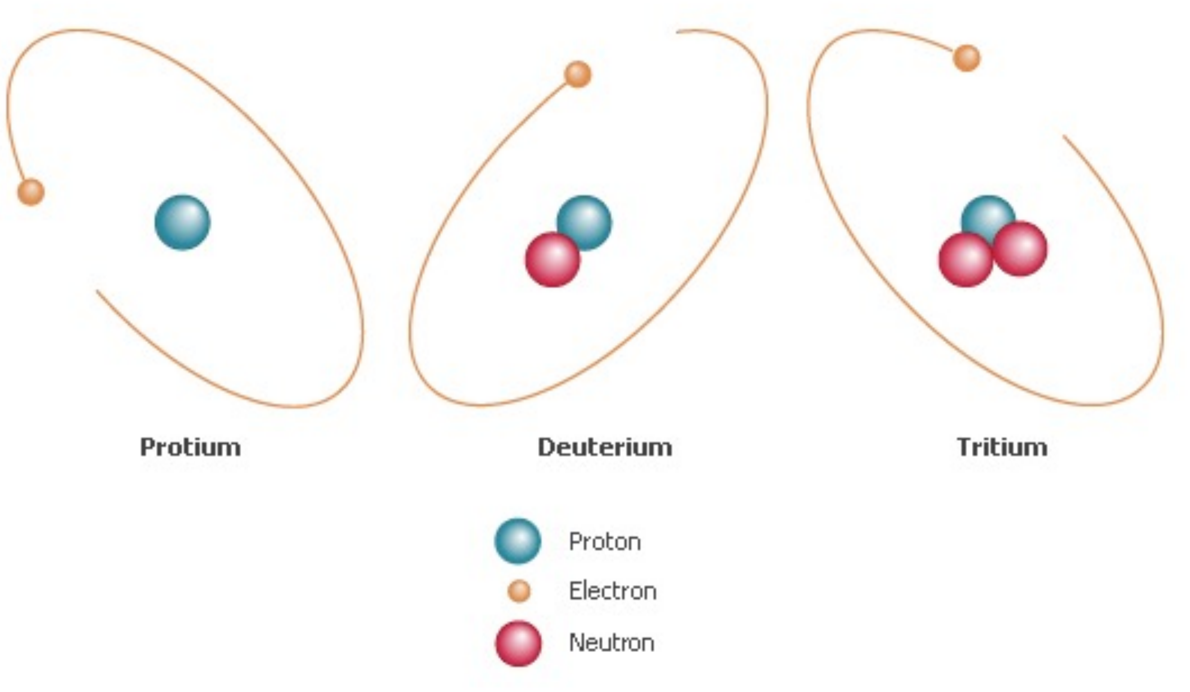
A =p+n

$_{2}{}^{4}He$

Z=p

Atoms are electrically neutral, i.e. they contain the same number of protons and electrons.

ISOTOPES = atoms with the same atomic number, but with different mass number.



Radioactive isotope

A =p+n

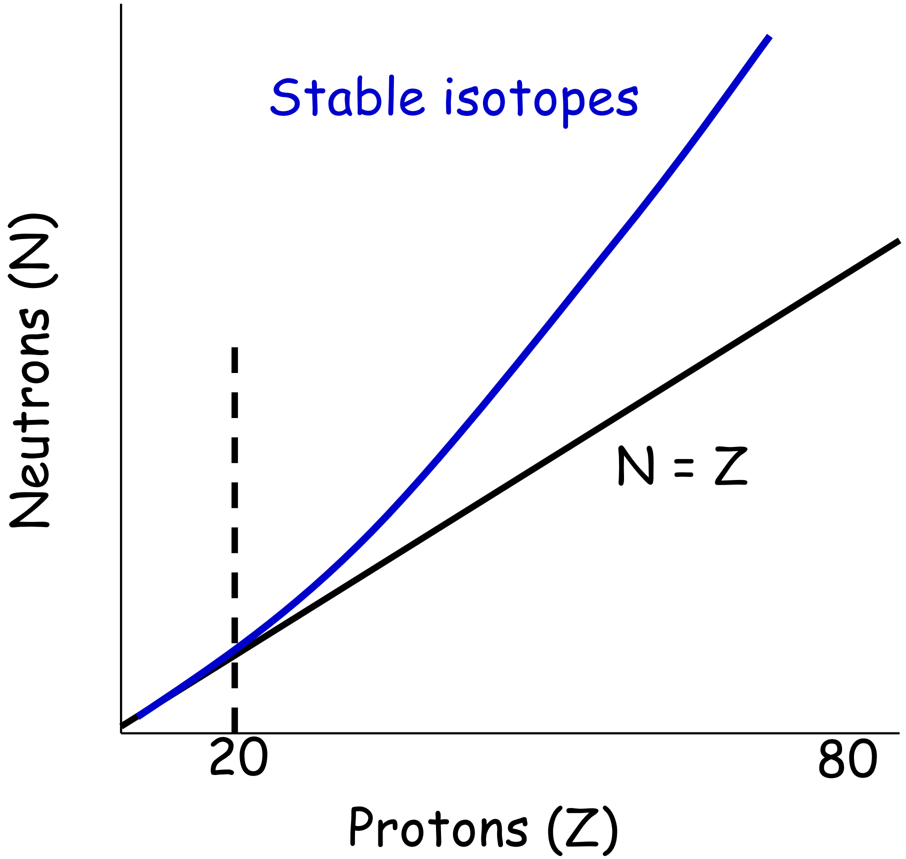
Z=p

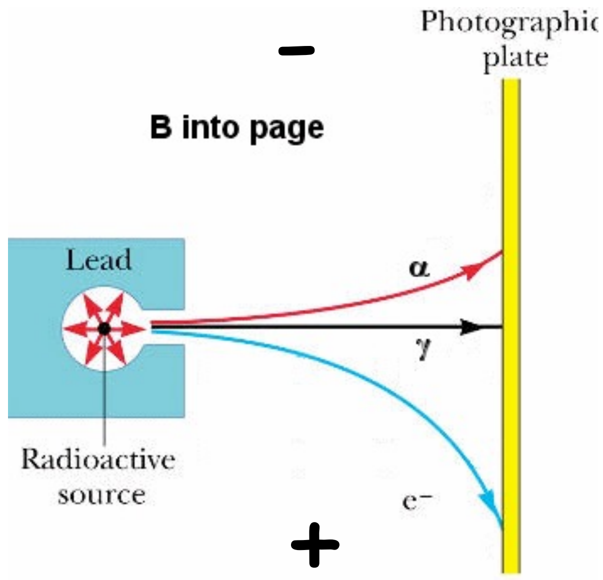
$^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$

STABILITY AND RADIOACTIVE DECAY OF NUCLEI

The composition of the nucleus in terms of protons and neutrons determines the stability of an element

Nuclei endowed with more than 84 protons are unstable.

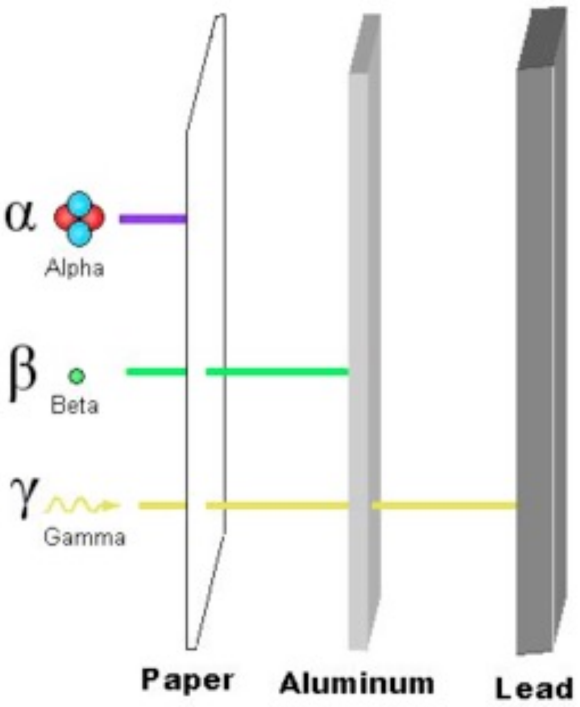




Magnetic field

EFFECT OF IONIZING RADIATION

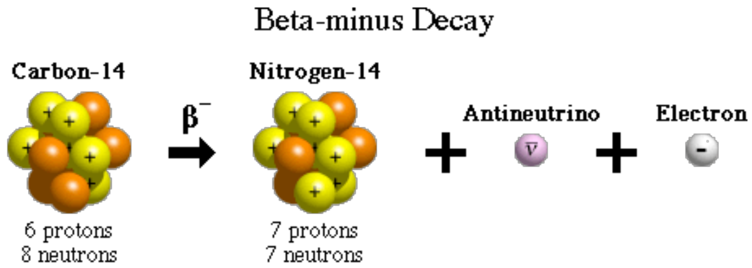
Ionizing radiation is the radiation generated by the decay of nuclei.
It has enough energy to ionize atoms/molecules, either directly (α and β particles) or indirectly (γ rays).



Radiation α: emission of 2 proton and 2 neutrons
Radiation β: emission of electrons
(induce transmutation)
Radiation γ: emission of high energy photons

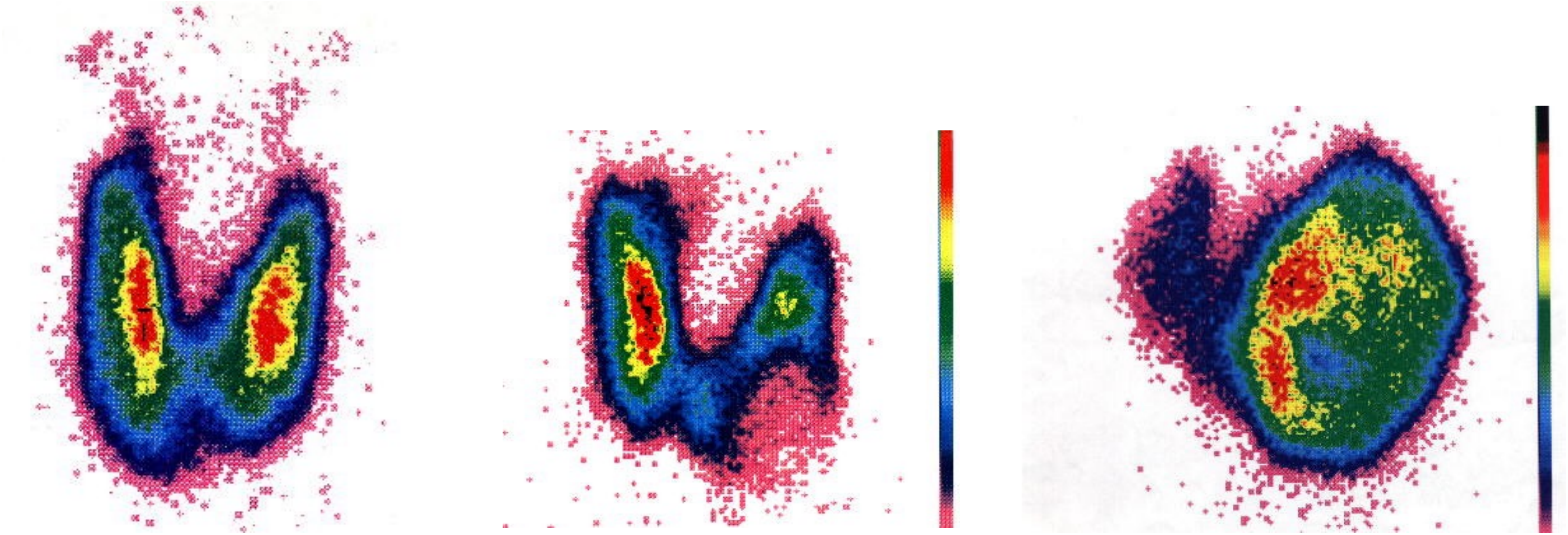
$$ {}^{3}_{1}H \rightarrow {}^{0}_{-1}\beta + {}^{3}_{2}He $$

$$ {}^{14}_{6}C \rightarrow {}^{0}_{-1}\beta + {}^{14}_{7}N $$



To reduce by 50% the intensity of gamma rays, 1 cm of lead, 6 cm of concrete or 9 cm of pressed material are required.

USE OF RADIOACTIVE ISOTOPES IN MEDICINE: THYROID SCINTIGRAPHY



$$^{131}I_{53} \rightarrow {}^{0}\beta_{-1} + {}^{131}Xe_{54}$$

What is the weight of an atom?

RELATIVE ATOMIC MASS

The reference is the mass of a stable and abundant isototope, ^{12}C

Atomic Mass Unit (AMU) =1/12 of the mass of the isotpe ^{12}C

1 AMU = $1.6605402 \times 10^{-27}$ kg

STANDARD ATOMIC WEIGHT: refers to the mean relative atomic mass of an element

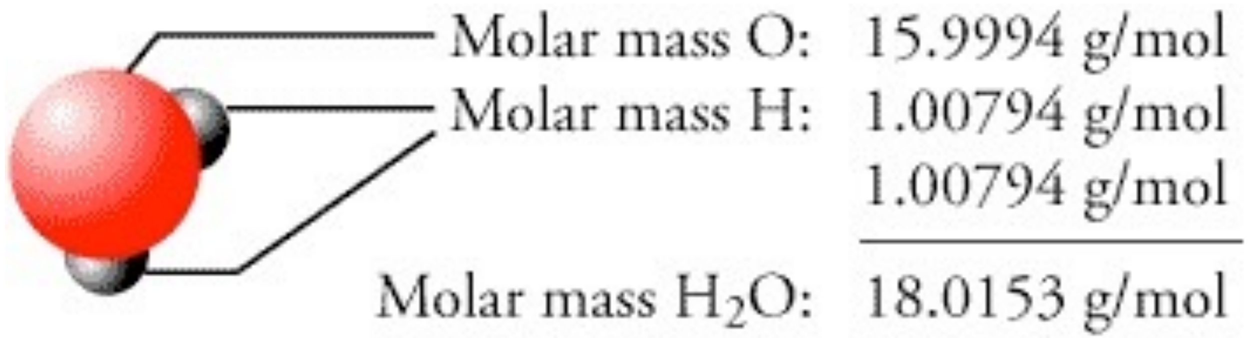
- For example, naturally occurring chlorine consists of atoms of *relative isotopic masses* 35 (75%) and 37 (25%). Its relative atomic mass is 35.5 a.m.u.

- $A_r = (75/100 \times 35) + (25/100 \times 37) = 35.5$

What is the weight of a compound?

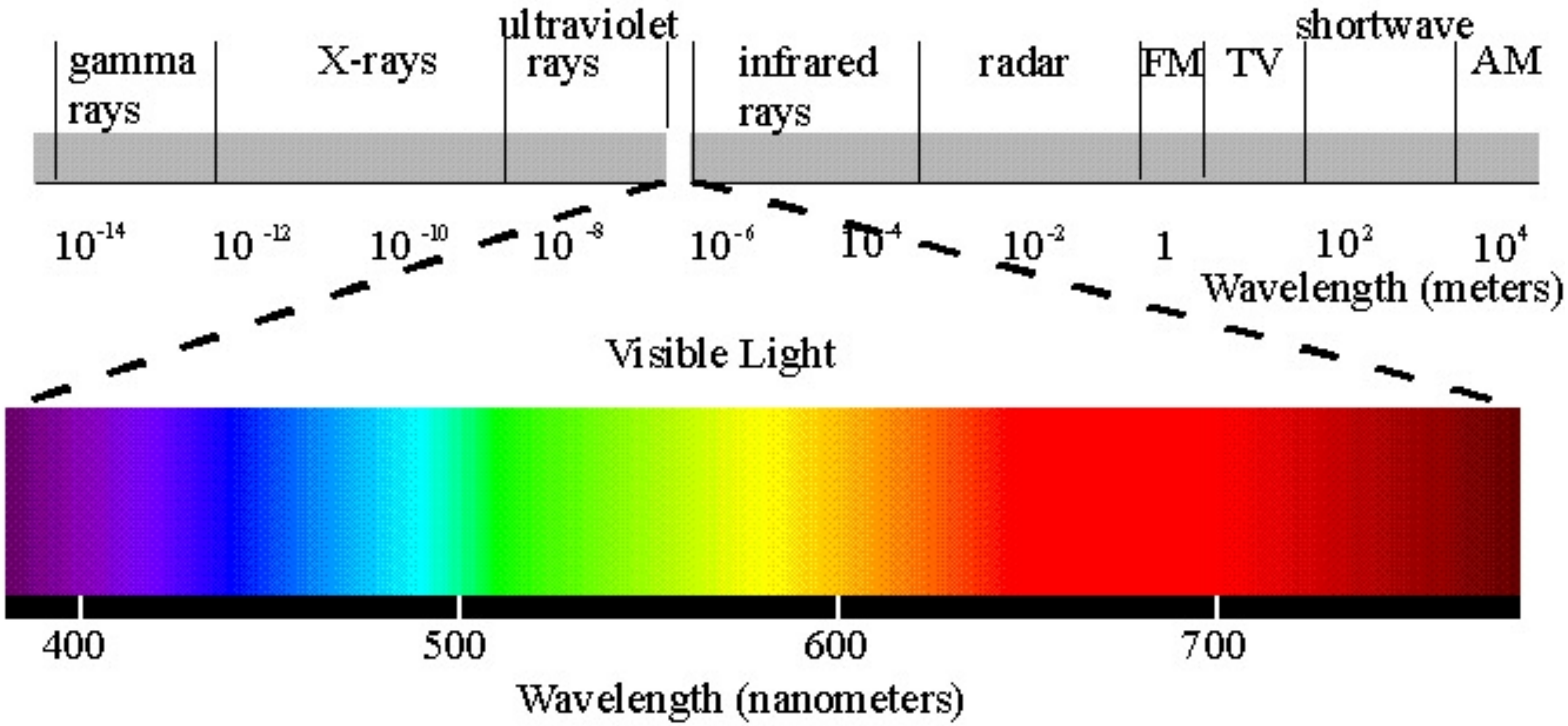
MOLECULAR WEIGHT

MW is the sum of the atomic weight of the elements in a compound multiplied by their coefficient, e.g. H_2O.

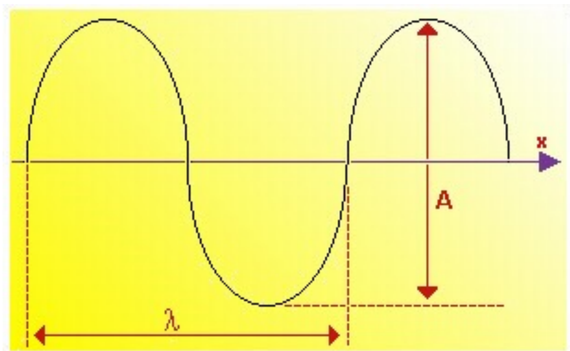


SPECTRUM OF ELECTROMAGNETIC RADIATION

Visible light is a part of the entire spectrum.
Energy increases as wavelength decreases
(increasing frequency). $c=\lambda x \nu$; $e=h\nu$.



c = speed of light
ν = frequency
h = Planck constant

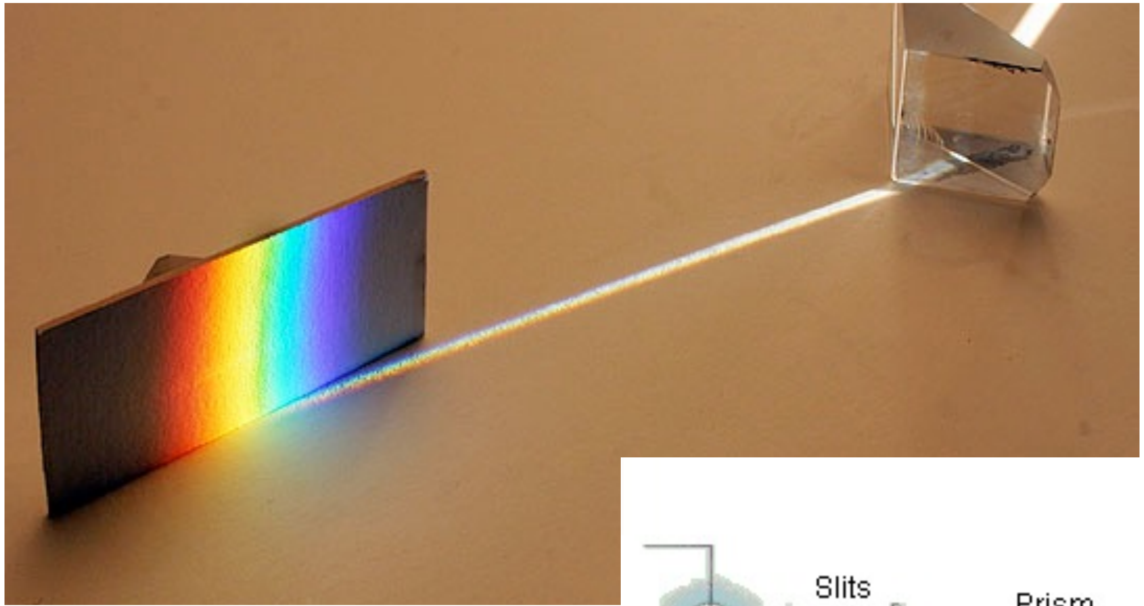


The Energy of a mole of photons: $h\nu N$

- A mole of red light photons (λ=865 nm) has an energy of 175 kJ
- For UV light E=300 kJ

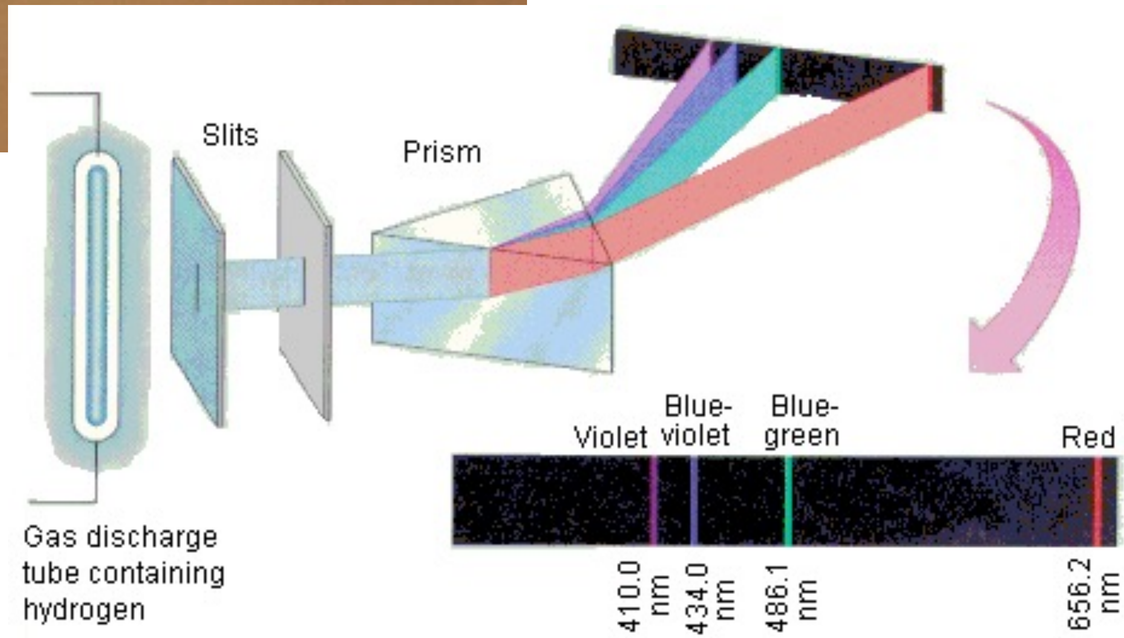
A "quantum" of light that can break DNA and protein chemical bonds.

N= Avogadro's number = $6{,}022 \cdot 10^{23}$

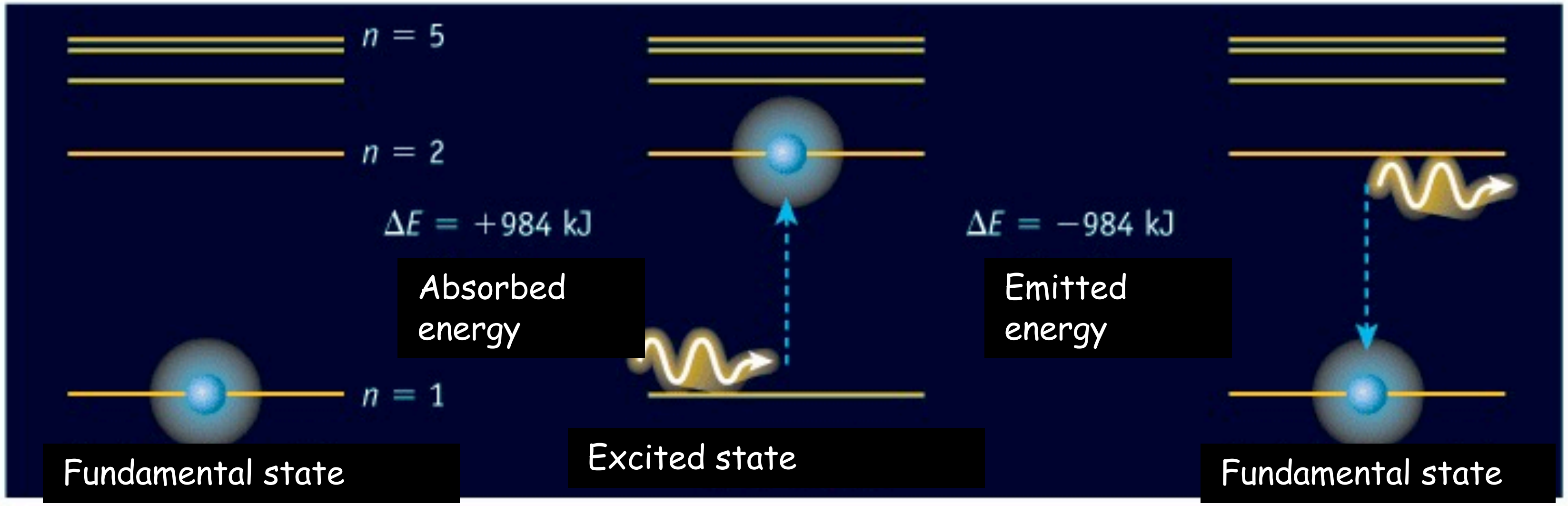


Sun light spectrum

Hydrogen lamp spectrum



The absorption and emission spectrum of hydrogen reveals the quantum nature of electron orbitals.



Energy absorption by an atom when it moves to an excited state.
When the electron moves from n=1 to n=2 the ΔE of energy is absorbed, which is emitted as it returns to the fundamental state.

Why atoms can be combined with each other and form molecules?

Electronic structure of the atom

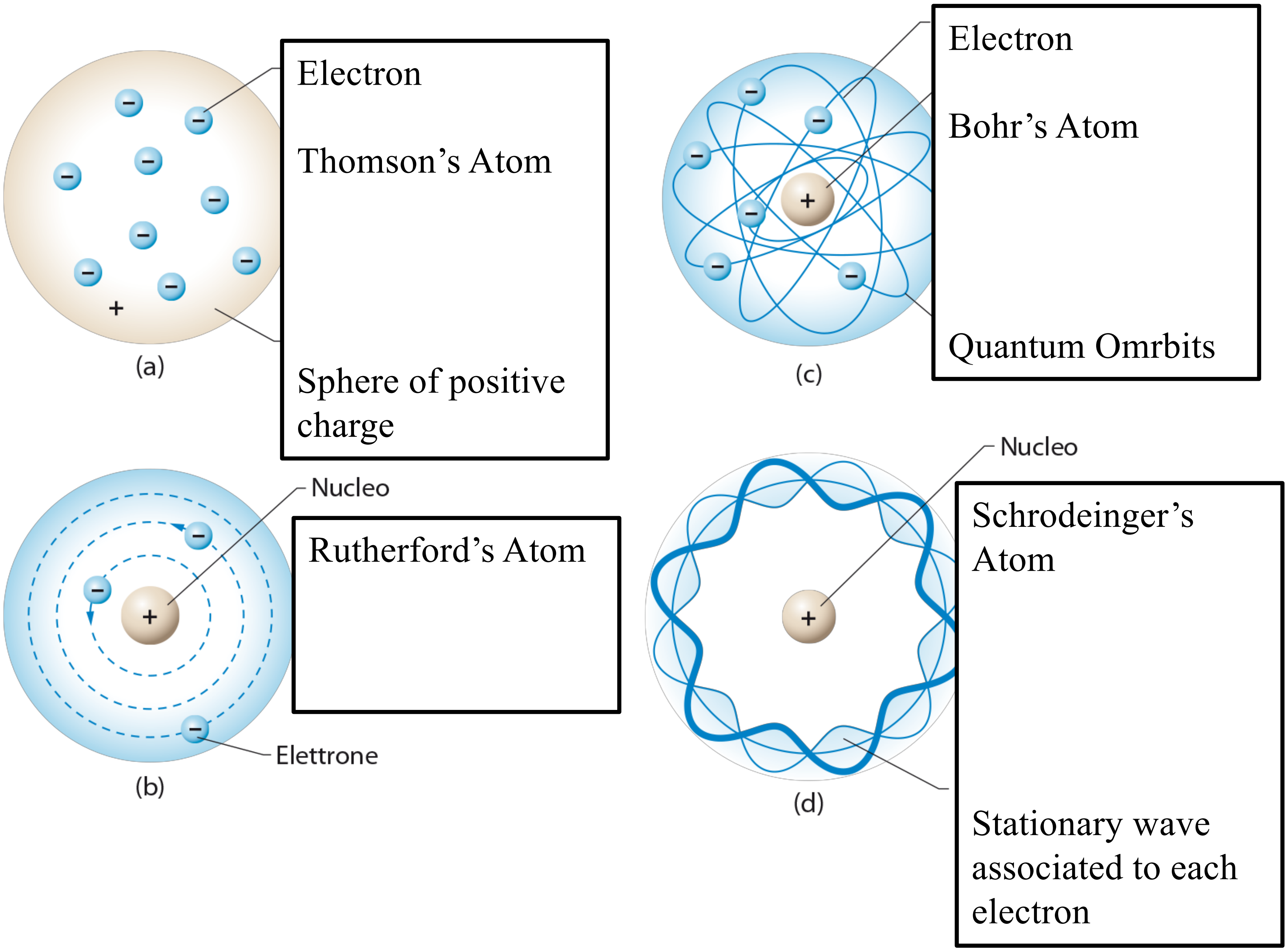
BOHR MODEL OF THE HYDROGEN ATOM (Z = 1 A = 1)

✓The electron moves around the central proton following circular orbits.

✓They are allowed orbits of a given radius related to an integer called principal quantum number n. Each orbit corresponds to an energy level (E).

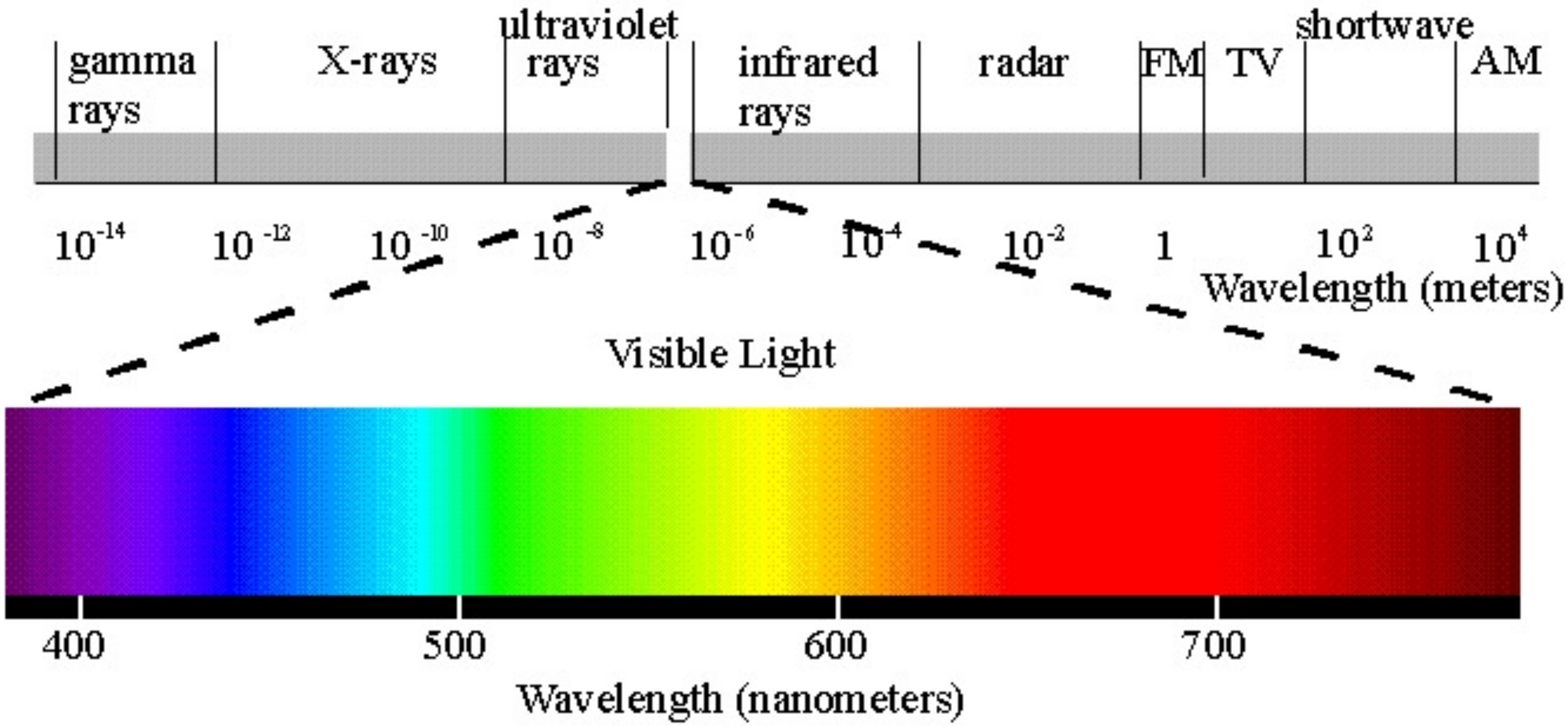
✓The electron is found in the orbit characterized by the lowest n and energy.

✓Following absorption of E the electron moves from one state to another. The absorbed energy corresponds exactly to the energy difference ΔE between the two allowed energy states.

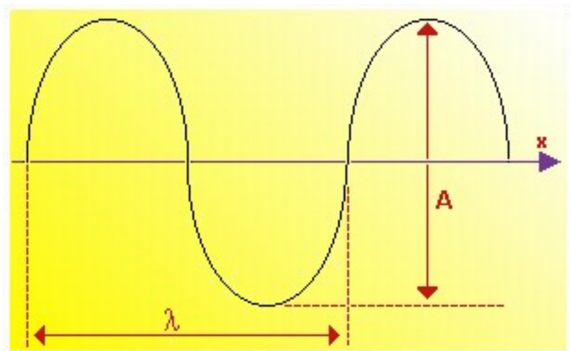

Electron
Thomson's Atom
Sphere of positive charge
(a)
Electron
Bohr's Atom
Quantum Omrbits
(c)
Nucleo
Rutherford's Atom
Elettrone
(b)
Nucleo
Schrodeinger's Atom
Stationary wave associated to each electron
(d)

SPECTRUM OF ELECTROMAGNETIC RADIATION

Visible light is a part of the entire spectrum.
Energy increases as wavelength decreases (increasing frequency). $c = \lambda \times \nu$; $e = h\nu$.



c = speed of light
ν = frequency
h = Planck constant



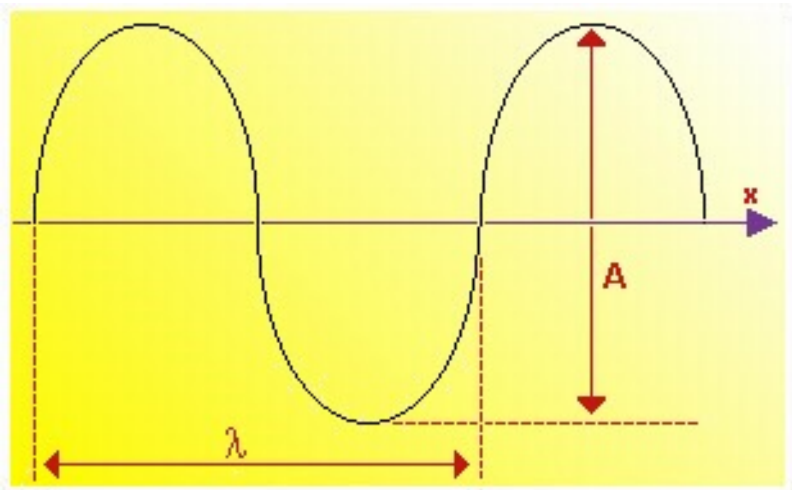
The photon: wave nature (electromagnetic radiation) and particle nature (Einstein's photoelectric effect) of matter.

Electrons moving in its circular orbit around the nucleus must be associated with a wavelength (λ) that depends on the mass of the particle (m) and velocity (v).

λ = **h/mv** De Broglie's equation

(h =Planck constant).

L.De Broglie
1892-1987



QUANTO-MECHANICAL DESCRIPTION OF THE ATOM

Mathematical description of the electron wave properties. The full quantum-mechanical description of an atom consists of a set of wave functions.

✓ The wave function Ψ describes the energy states accessible to electrons.

$$\frac{\delta^2 \psi}{\delta x^2} + \frac{\delta^2 \psi}{\delta y^2} + \frac{\delta^2 \psi}{\delta z^2} + \frac{8 \pi^2 m}{h^2} (E - V) \quad \psi = 0$$

Schrodinger's equation

✓The allowed energy states coincide with those predicted by the Bohr model, however, for the uncertainty principle, you can not specify both the position and velocity of a particle. $\Delta x \Delta p \geq \frac{\hbar}{2}$

✓The probability for the electron to be found in a given position around the nuclues is $= \Psi^2$

ORBITALS

Each wave function which describes the motion of an electron corresponding to a given energy level is called an atomic orbital.

The model implies 3 quantum numbers (n, l, m) that characterize each orbital.

✓ Principal quantum number *n* : depends on the distance from the nucleus. It defines the energy level. It is an integer (1, 2 ,3…).

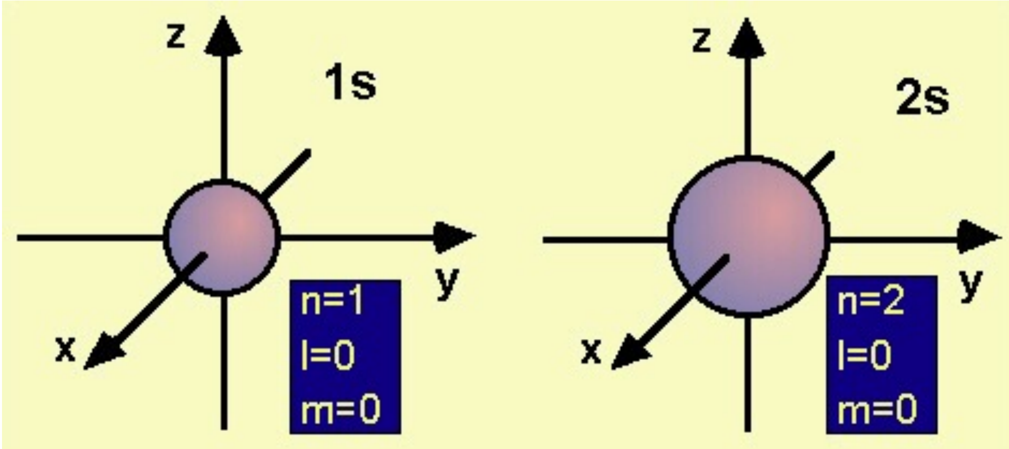
✓ Azymuthal quantum number *l*: determines the shape of the orbital, it ranges from 0 to n-1.

l	**0**	**1**	**2**	**3**	**4**
Orbital	**s**	**p**	**d**	**f**	**g**

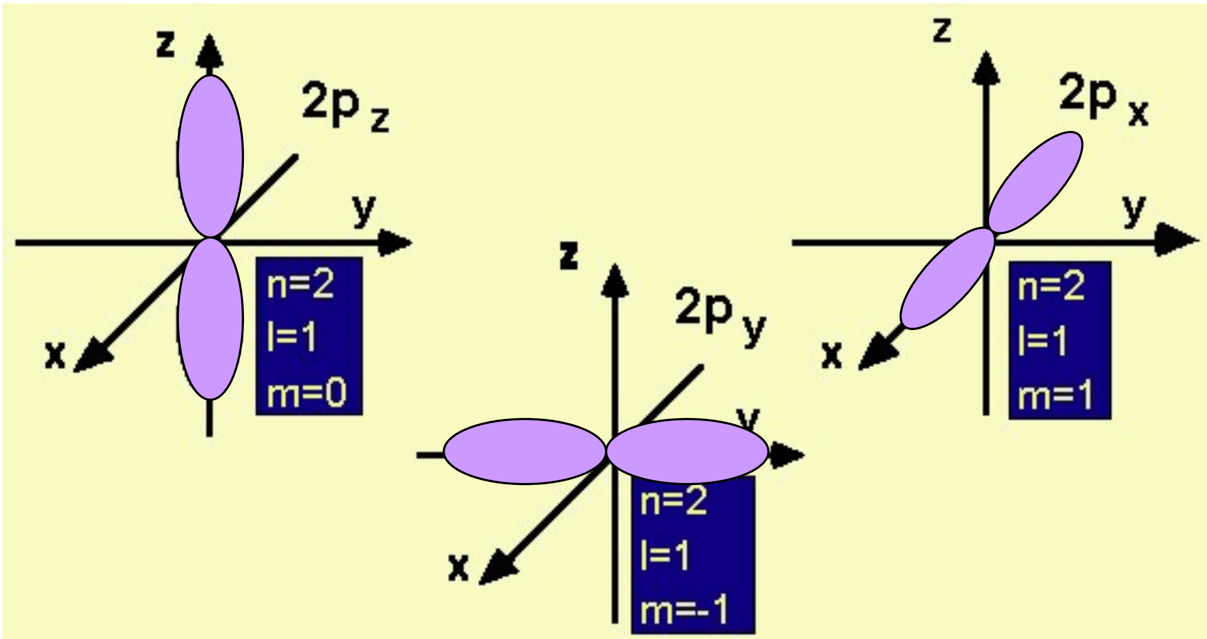
✓ Magnetic quantum number *m*: it ranges from –l to +l .
It determines the orientation of the orbital.

Shape of the orbitals

s type orbitals



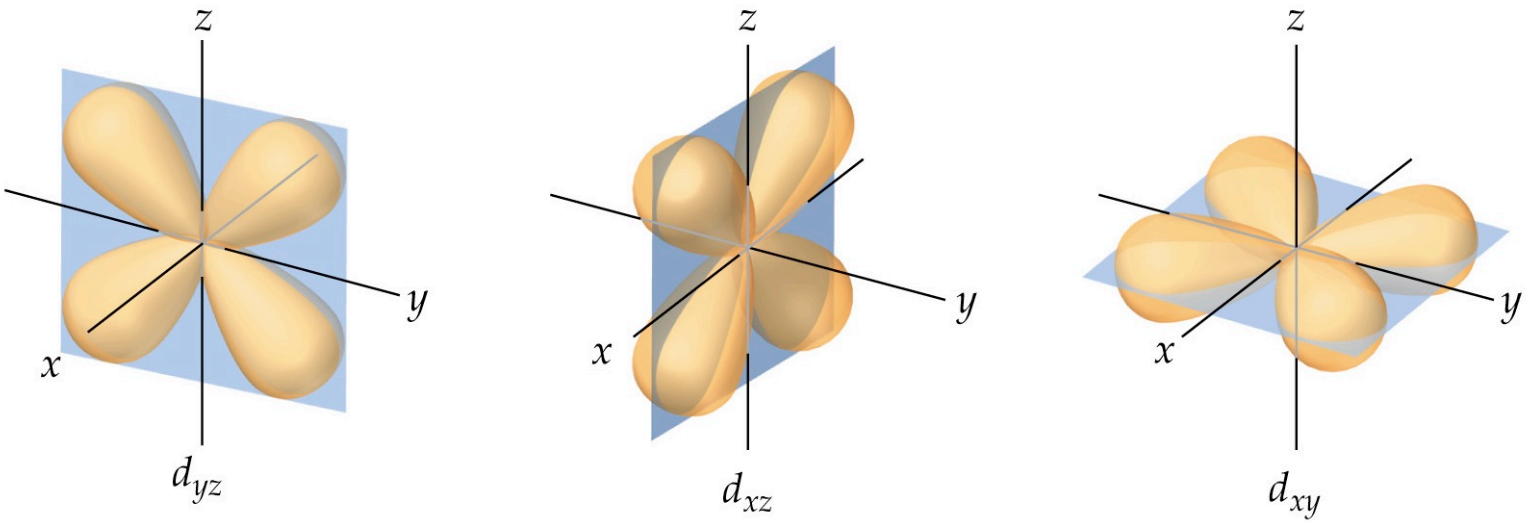
p type orbitals

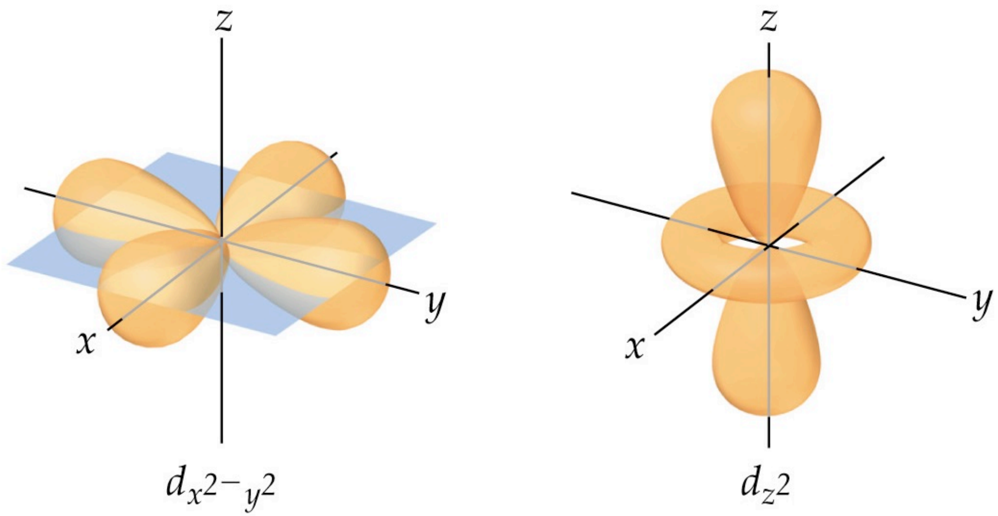


n = 1, 2, 3…

l = from 0 to n-1

m = from – *l* to *l*





n = 3

l = 2

m = from – *2* to *2*

d type orbitals

n	l	m	orbital: s	orbital: p	orbital: d
1	0	0	1s		
2	0	0	2s		
2	1	0		$2p_z$	
2	1	1		$2p_x$	
2	1	-1		$2p_y$	
3	0	0	3s		
3	1	0		$3p_z$	
3	1	1		$3p_x$	
3	1	-1		$3p_y$	
3	2	0			$3d_z2$
3	2	1			$3d_{xz}$
3	2	-1			$3d_{yz}$
3	2	2			$3d_{xy}$
3	2	-2			$3d_x2_{-y}2$

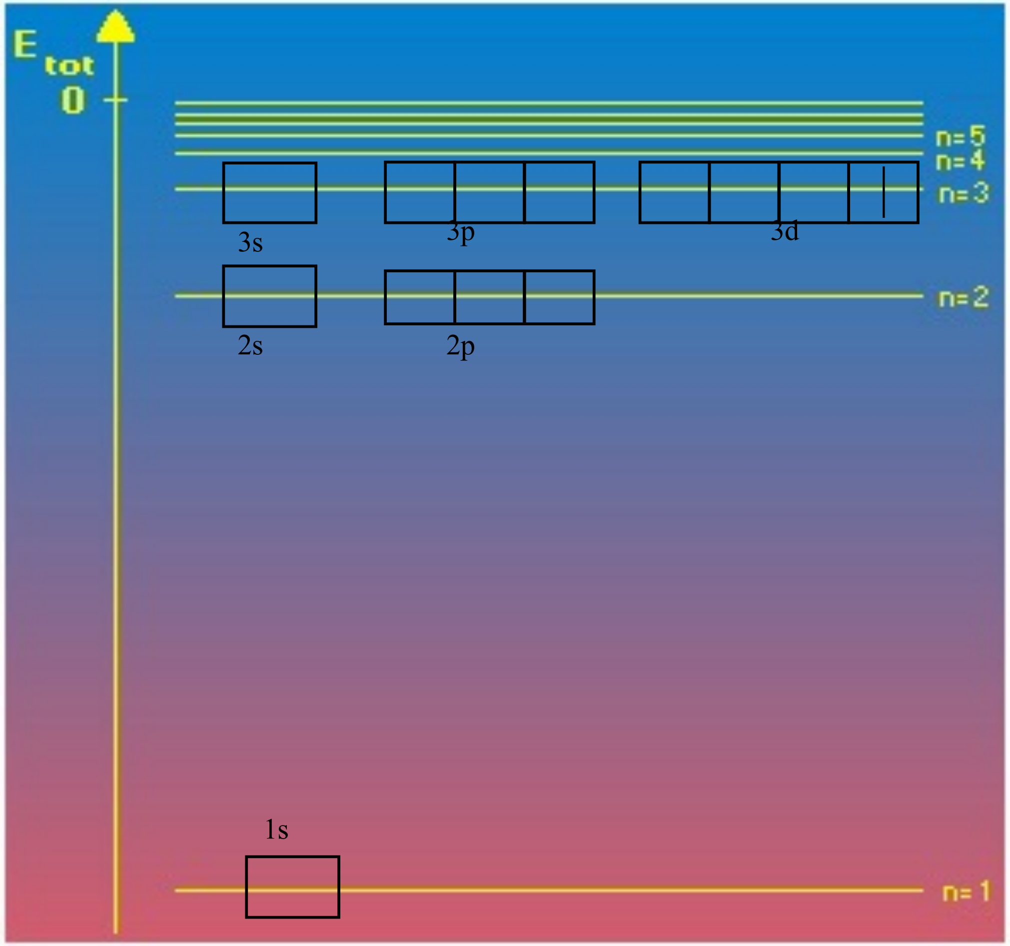
n = 1, 2, 3…

l = from 0 to n-1

m = from – l to l

Diagram of orbital energy levels in an one-electron atom (H)

All orbitals having the same value of n (principal quantum number) have the same energy



Excited states

Fondamental state

The fourth quantum number: electronic spin

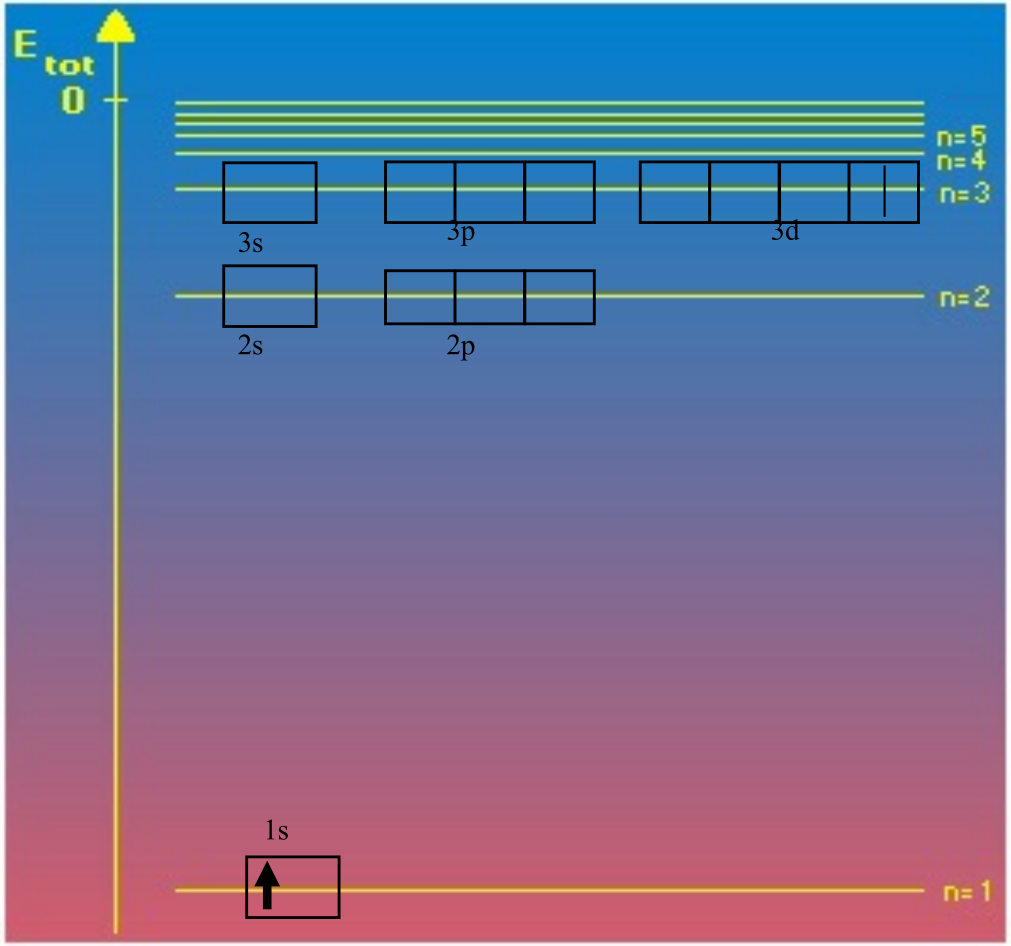
The spin quantum numenber s : describes the spin of the electron within that orbital. It can have two values: +1/2 and –1/2.

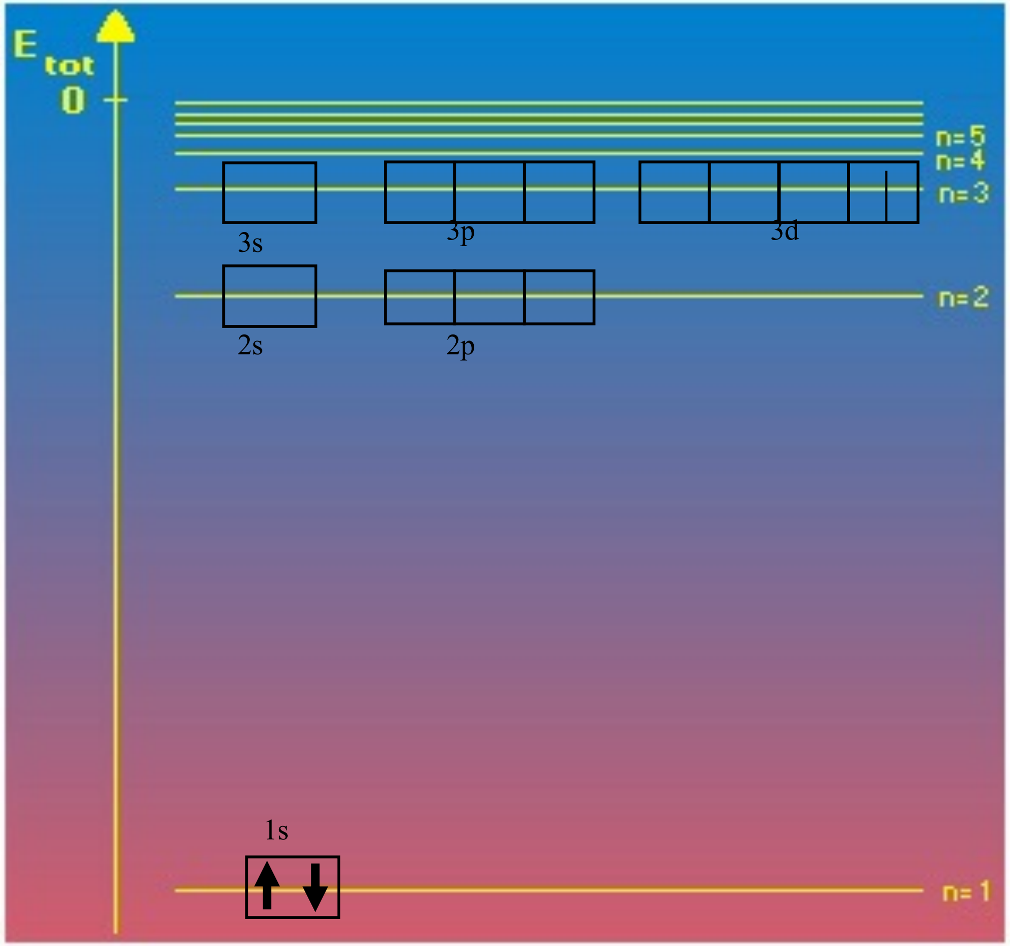
The **AUFBAU** principle (in German "building up") is used to determine the electron configuration of an atom, by adding electrons around the nucleus in the most stable energy level.

Principle of minimum energy: each electron occupies the available orbital with the lowest energy level.

Pauli exclusion principle: in an atom it is not allowed to have two electrons which possess identical quantum numbers. So an orbital can be occupied by two electrons with different spin number.

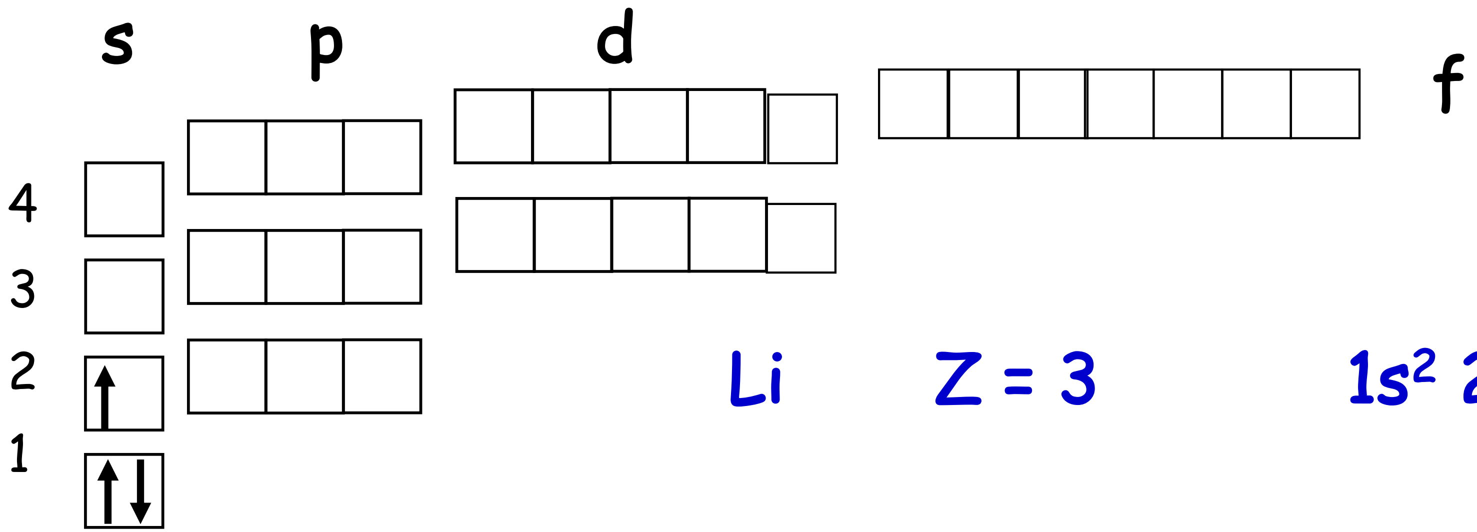
Hund Principle : if two or more electrons occupy isoenergetic orbitals, they fill the empty ones first, with parallel spin.



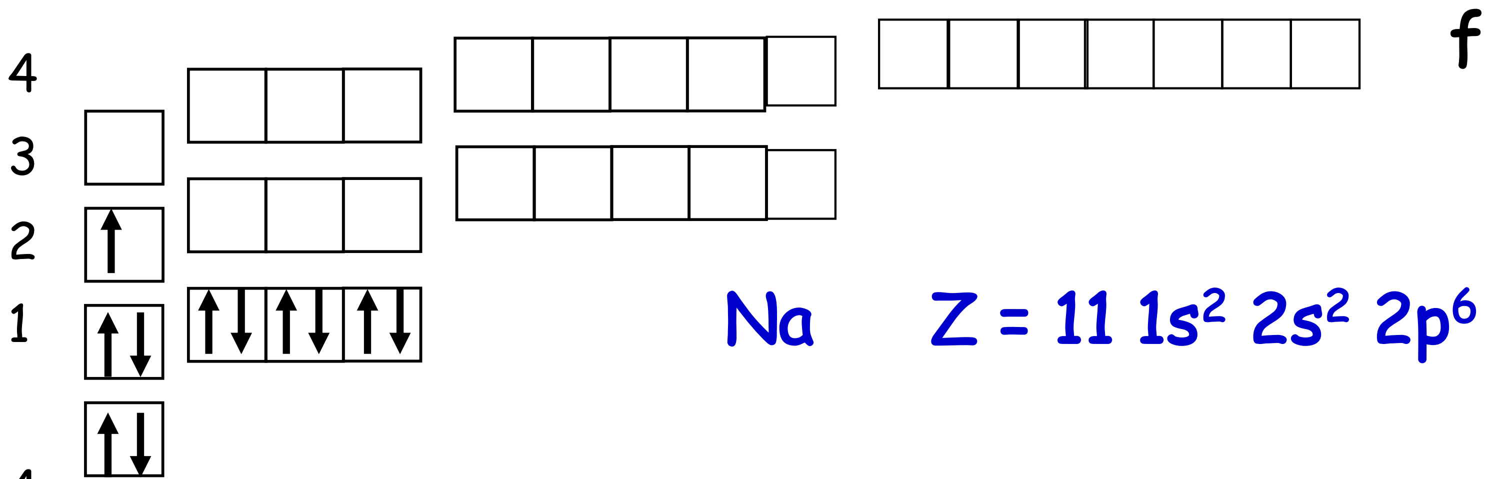


H; Z = 1 $1s$

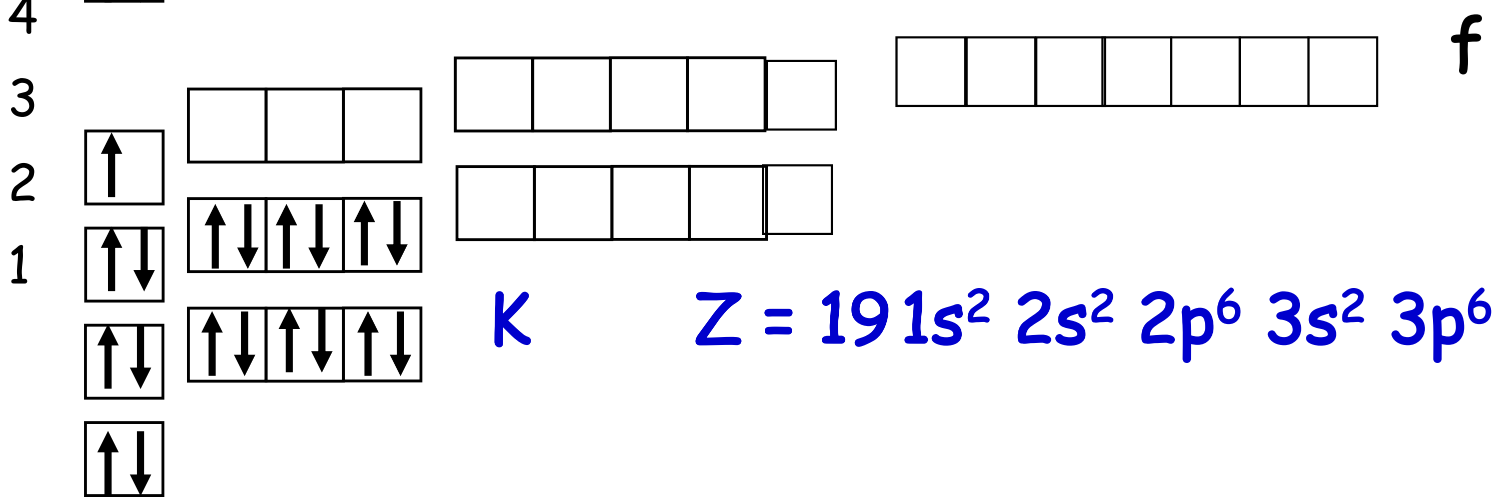
He; Z =2 $1s^2$



Li $Z = 3$ $1s^2\ 2s$



Na $Z = 11$ $1s^2\ 2s^2\ 2p^6\ 3s$



K $Z = 19$ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s$

Z	Symbol/e^-	Electronic configuration	
3	Li	(He) 2s ↑	$1s^2 2s^1$
4	Be	(He) 2s ↑↓	$1s^2 2s^2$
5	B	(He) 2s ↑↓ 2p ↑	$1s^2 2s^2 2p^1$
6	C	(He) 2s ↑↓ 2p ↑ ↑	$1s^2 2s^2 2p^2$
7	N	(He) 2s ↑↓ 2p ↑ ↑ ↑	$1s^2 2s^2 2p^3$
8	O	(He) 2s ↑↓ 2p ↑↓ ↑ ↑	$1s^2 2s^2 2p^4$
9	F	(He) 2s ↑↓ 2p ↑↓ ↑↓ ↑	$1s^2 2s^2 2p^5$
10	Ne	(He) 2s ↑↓ 2p ↑↓ ↑↓ ↑↓	$1s^2 2s^2 2p^6$
11	Na	(Ne) 3s ↑	$1s^2 2s^2 2p^6 3s^1$

ELECTRONIC CONFIGURATION AND CLASSIFICATION OF THE ELEMENTS

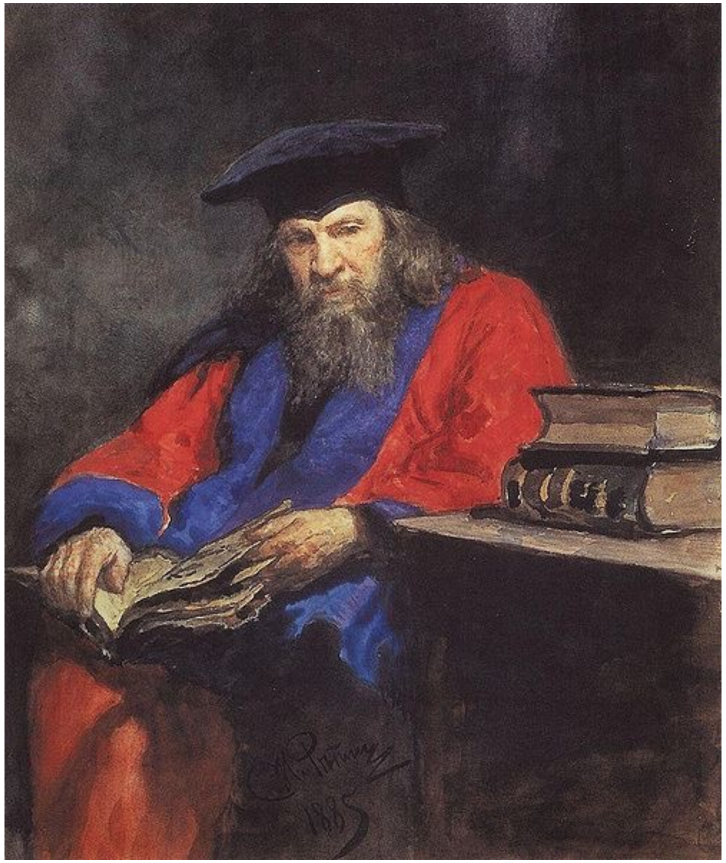
The discovery of several new elements in the nineteenth century had as a natural consequence several attempts of a classification.

Mendeleev arranged the elements in order of increasing atomic number Z, highlighting the periodic nature of their chemical and physical properties (Periodic Table).

Groups (table columns): elements that have the same external electronic configuration.

Periods (table rows): start with an element that has the outer electron configuration of 1s electron and continues by increasing the atomic number. The external electrons have the same quantum number n.

Dmitri Mendeleeiev formulated the PeriodicTable of Elements in 1869.
Unlike other contributors to the table, Mendeleev provided a classification system that could predict the characteristics of elements not yet discovered.



Dmitri Mendeleev born inTobolsk,
Siberia (1834-1907).

He resigned from the University August 17, 1890,
when the Russian government rejected a draft reform of the curriculum presented by his students.

ELECTRONIC CONFIGURATION AND CLASSIFICATION OF THE ELEMENTS

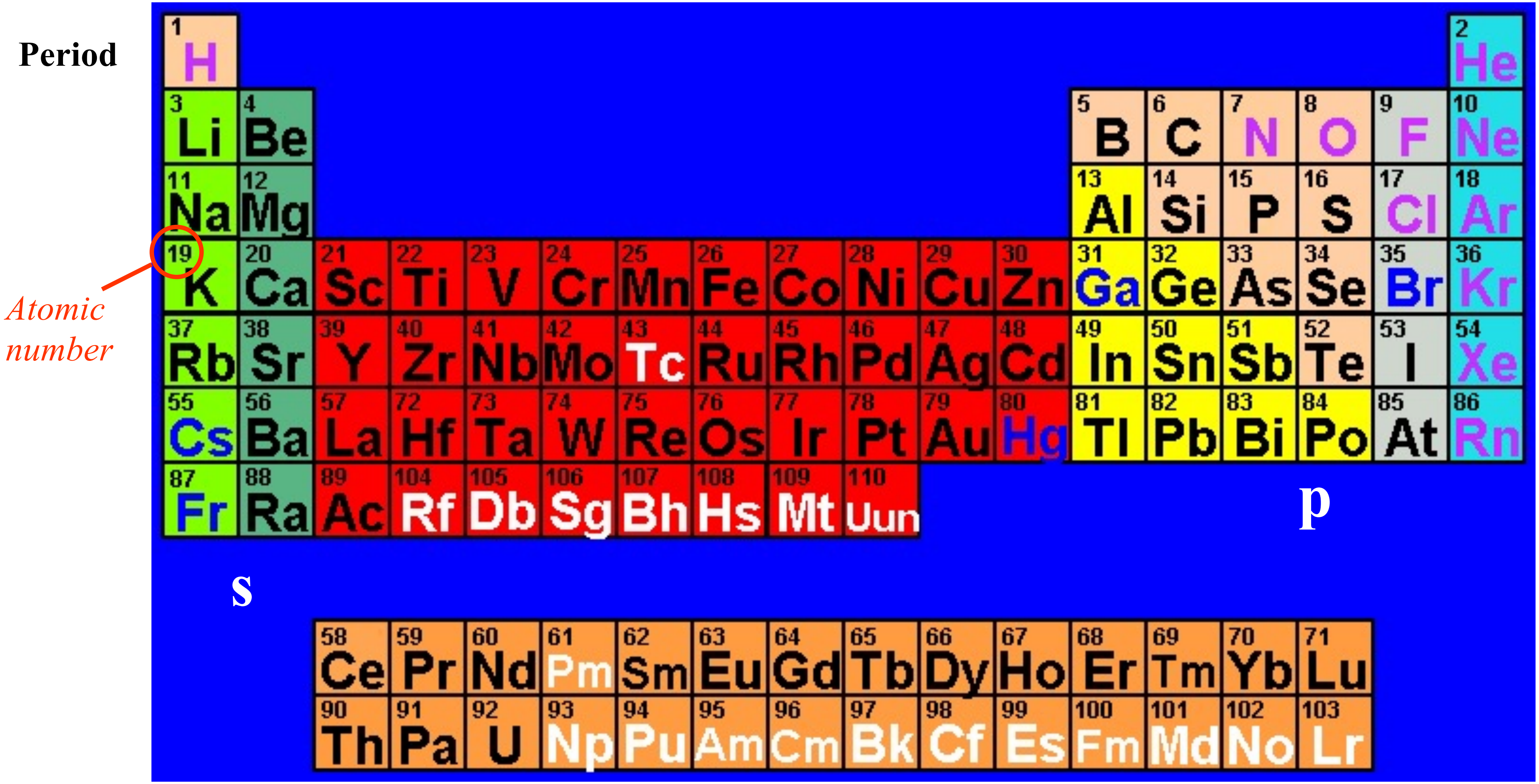
Mendeleev arranged the elements in order of increasing atomic number Z, highlighting the periodic nature of their chemical and physical properties (Periodic Table).
He predicted the existence of new elements, the usage of the atomic weight (and not the number) made rationalization very difficult.

	Gruppe I. R^1O	Gruppe II. RO	Gruppe III. R^1O^3	Gruppe IV. RH^4 RO^7	Gruppe V. RH^3 R^2O^5	Gruppe VI. RH^3 RO^3	Gruppe VII. RH R^2O^7	Gruppe VIII. — RO^4
1	H = 1							
2	Li = 7	Be = 9.4	B = 11	C = 12	N = 14	O = 16	F = 19	
3	N = 23	Mg = 24	Al = 27.3	Si = 28	P = 31	S = 32	Cl = 35.5	
4	K = 39	Ca = 40	— = 44	Ti = 48	V = 51	Cr = 52	Mn = 55	Fe = 56 Co = 59 Ni = 60, Cu = 63.
5	(Cu = 63)	Zn = 65	— = 68	— = 72	As = 75	Se = 78	Br = 80	
6	Rb = 85	Sr = 87	?Yt = 88	Zr = 90	Nb = 94	Mo = 56	— = 100	Ru = 104, Rh = 104, Pd = 106, Ag = 104.
7	(Ag = 104)	Cd = 112	In = 113	Sn = 118	Sb = 122	Te = 125	J = 127	
8	Cs = 133	Ba = 137	?Di = 138	?Ce = 140	—	—	—	— — — —
9	)—)	—	—	—	—	—	—	
10	—	—	?Er = 178	?La = 180	Ta = 182	W - 184	—	Os = 195, Ir = 197, Pt = 198, Au = 199.
11	(Au = 199)	Hg = 200	Tl = 204	Pb = 207	Bi = 208	—	—	
12	—	—	—	Th = 231	—	U = 240	—	— — — —

Mendeleev's Periodic Table of 1871, redrawn by J. O. Moran, 2013

Periodic table of the elements

Group



Metals

Alkali Metals

Transition elements: orbitals *d* and *f* are filled.

Halogens

Noble Gases

http://periodic.lanl.gov/default.htm

Scene from "The Big Bang Theory" on CBS

http://www.webelements.com/

How are the electrons arranged arranged in the orbitals of the elements of the periodic table?

n = 1

Fundamental state: electrons in the minimum energy level.

The 1s orbital (n = 1, l = 0, m = 0) is the orbital with the lowest energy.

Pauli principle, construction of H ($1s^1$) e He ($1s^2$)

As the orbital with n = 1 is full

n = 2

The next orbital with lower energy after 1s is populated, 2s (Li = $1s^22s$): new shell, new period (Be = $1s^22s^2$)

Element	n. of electrons	Electronic configuration
H	1	$1s^1$
He	2	$1s^2$
Li	3	$1s^22s$
Be	4	$1s^22s^2$
B	5	$1s^22s^22p$
C	6	$1s^22s^22p^2$

Hund principle: the electrons arrange themselves occupying all degenerate orbitals available

Groups are made of elements with the same outer electron configuration.

Metals (Group I):

Element	n. electrons	Electronic confguration
Li	3	$1s^2 2s$
Na	11	$1s^2 2s^2 2p^6 3s$
K	19	$1s^2 2s^2 2p^6 3s^2 3p^6 4s$

Alkali metals (Group II)

Element	n. electrons	Electronic confguration
Be	4	$1s^2 2s^2$
Mg	12	$1s^2 2s^2 2p^6 3s^2$
Ca	20	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

halogens (Group VII)

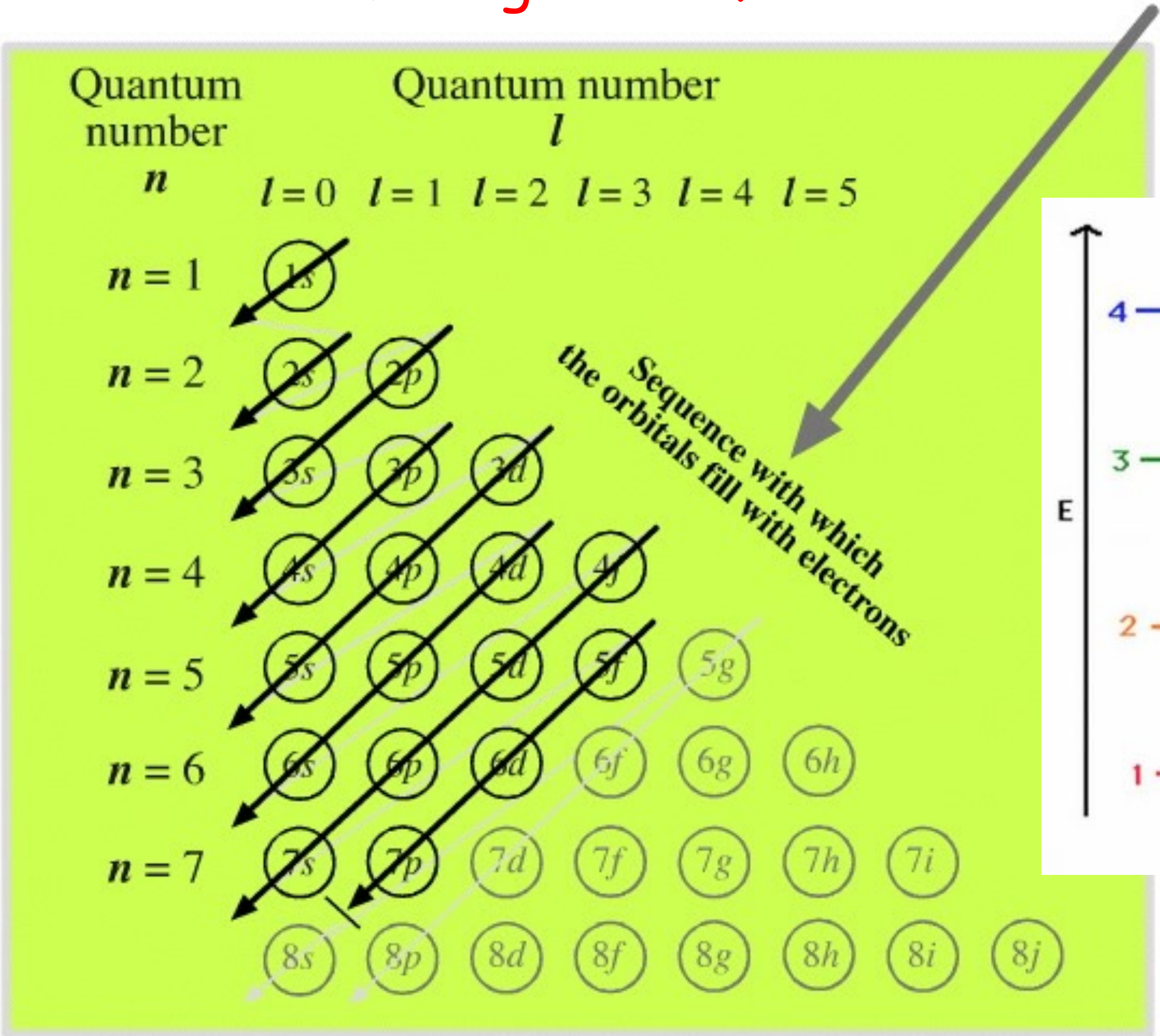
Element	n. electrons	Electronic confguration
F	9	$1s^2 2s^2 2p^5$
Cl	17	$1s^2 2s^2 2p^6 3s^2 3p^5$

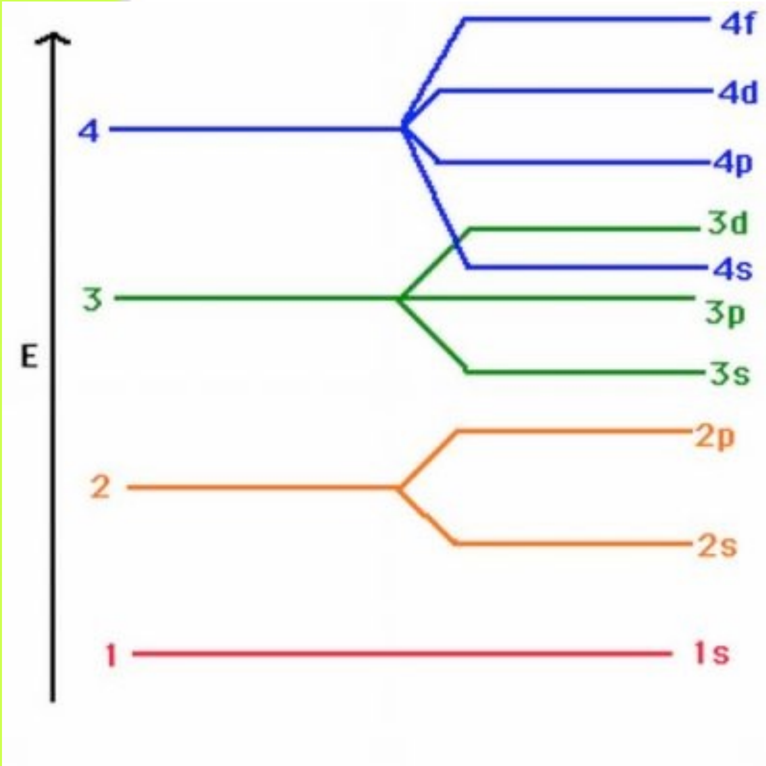
Noble gases (Group 0)

The configuration corresponding to the total filling of the orbital s and p by 8 electrons, in an extremely stable one (elements with high ionization energy, low electron affinity and non-reactive).

Element	**n. electrons**	**Electronic confguration**
Ne	10	$1s^2 2s^2 2p^6$
Ar	18	$1s^2 2s^2 2p^6 3s^2 3p^6$

Filling order for orbitals





Orbitals are filled with increasing n + l. For a given n + l, the one with the lowest n will be filled first

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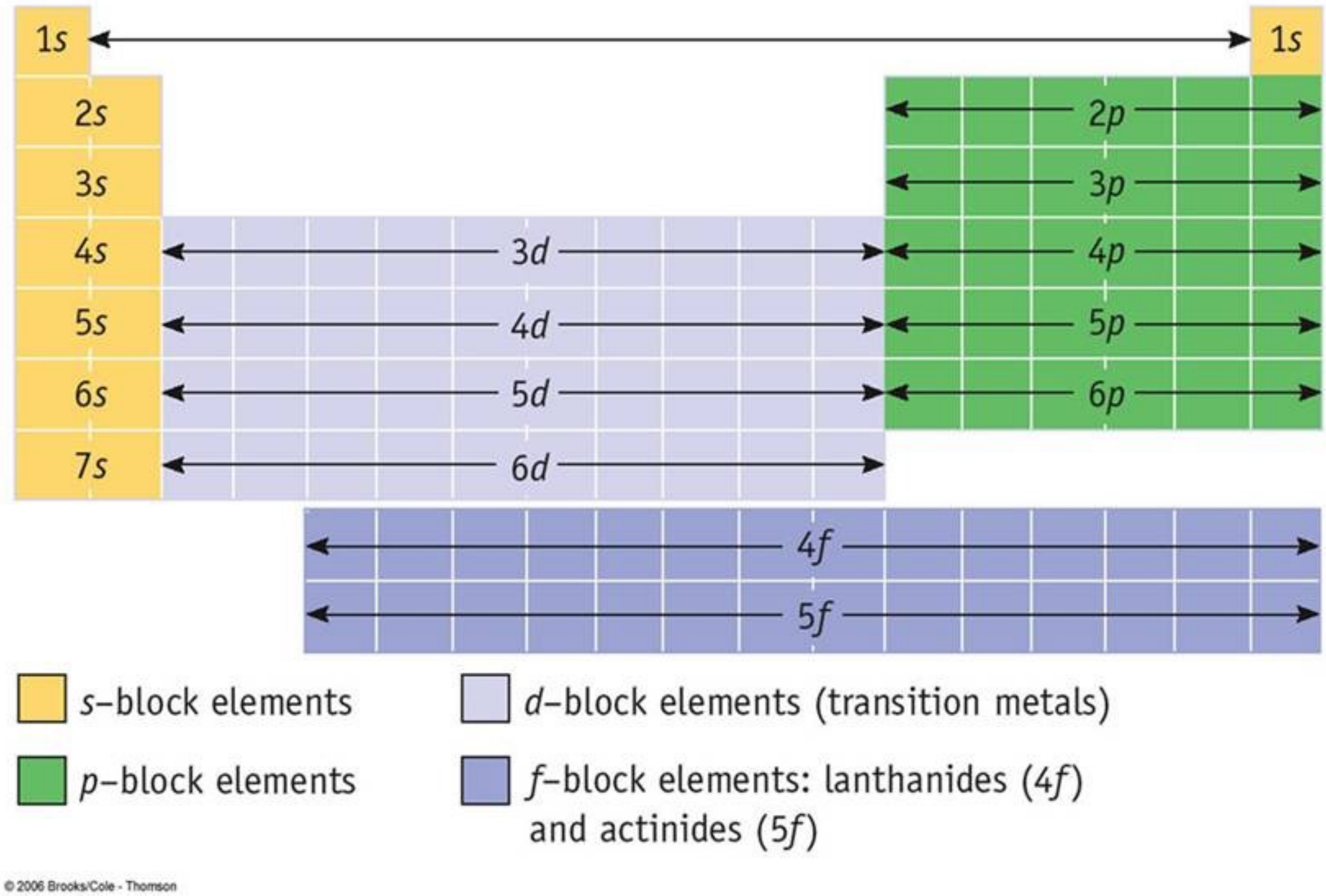
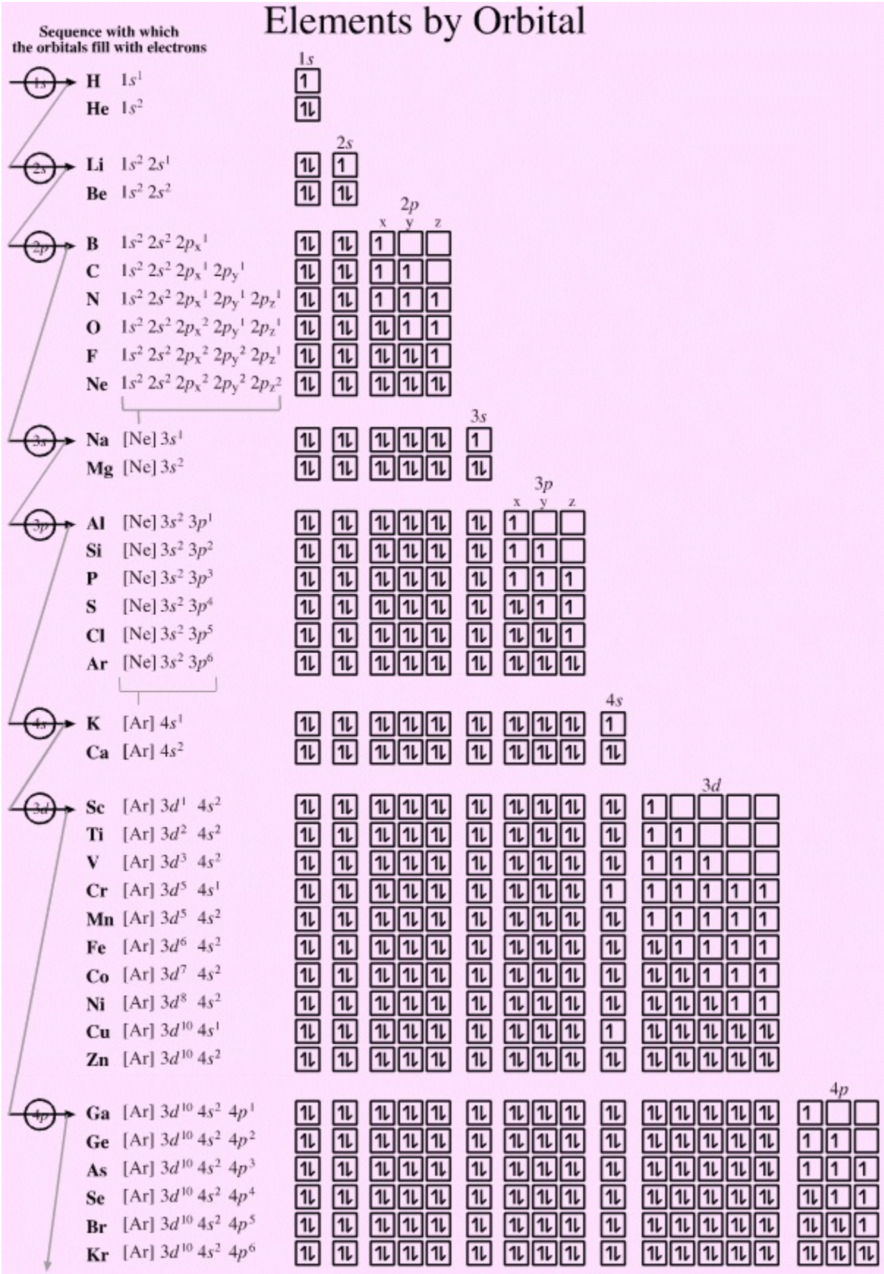


Filling order for orbitals and periodic table



Elements and their electronic configuration.

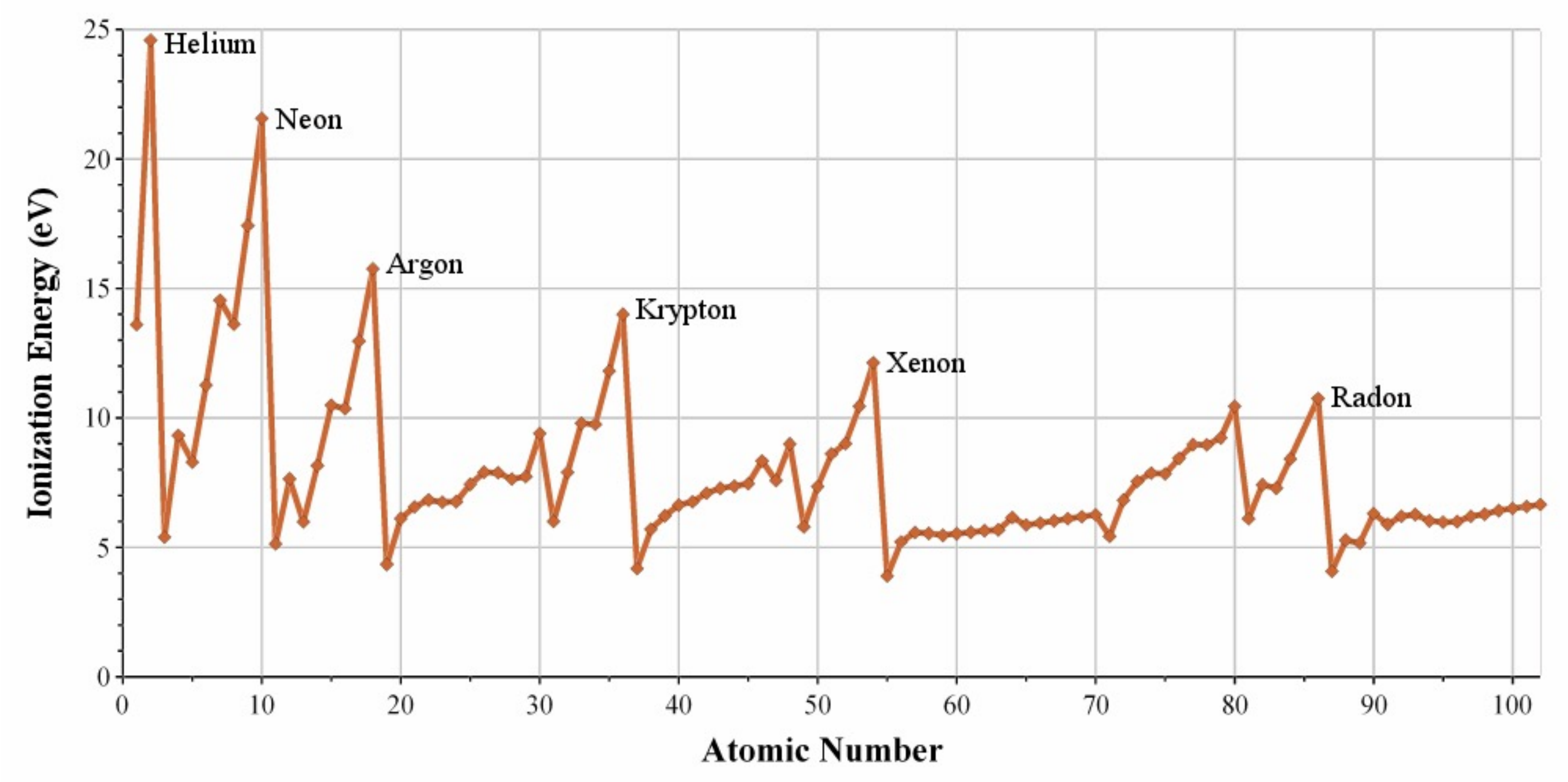
Ionization Energy (I)

It is the energy required to remove an electron from an atom or an ion.

$X \rightarrow X^+ + e^-$ First ionization energy

$X^+ \rightarrow X^{++} + e^-$ Second ionization energy

It is related to the attraction of the electron in the atom or ion.
It increases for each subsequent electron to be removed (the screening effect of electrons decreases).
It increases moving towards the right along a period, it decreases going towards the bottom of a group.



Periodicity of the ionization energy.

Electron affinity

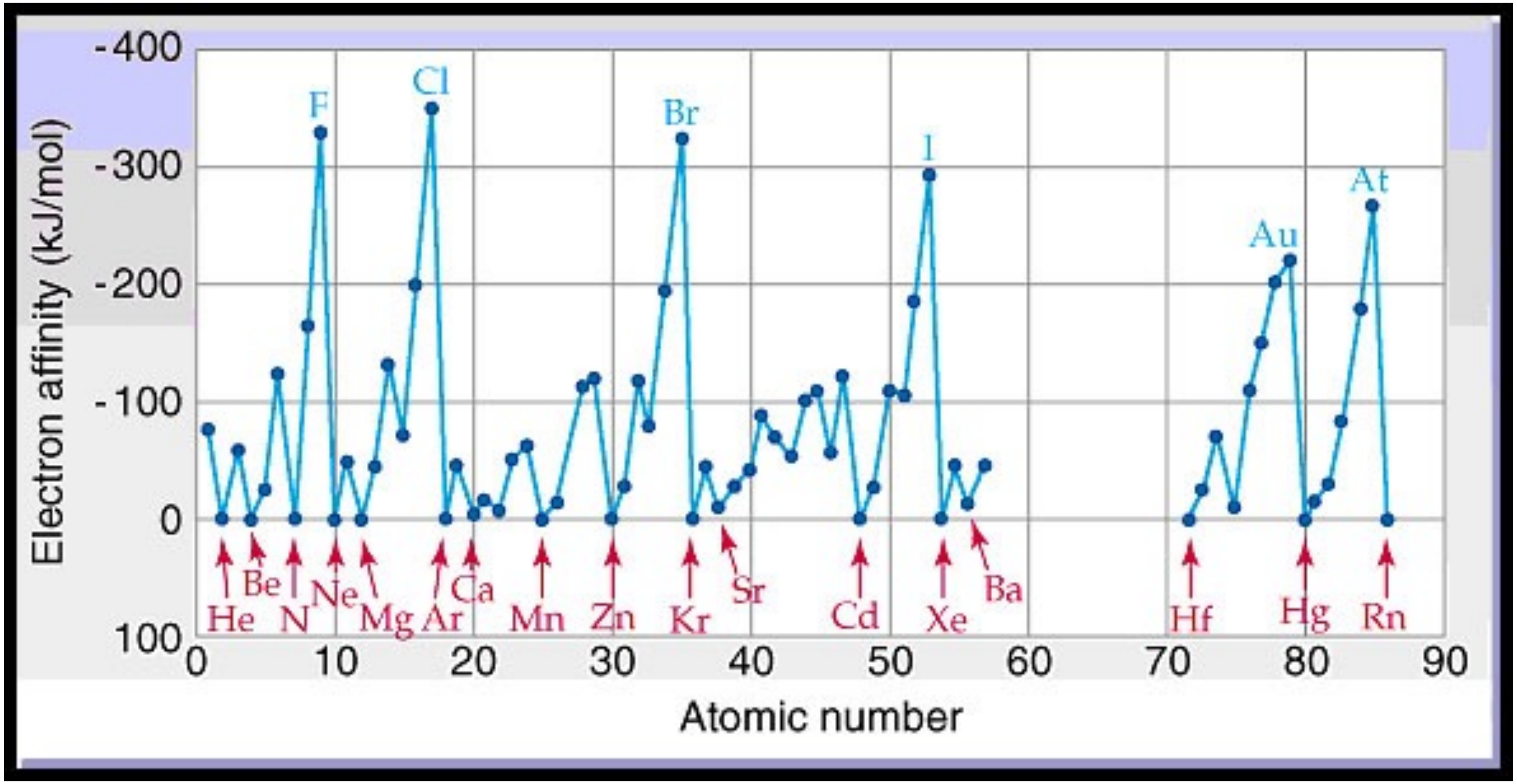
It is the energy associated with the process of addition of an electron to an atom or an ion.

$X + e^- \rightarrow X^-$

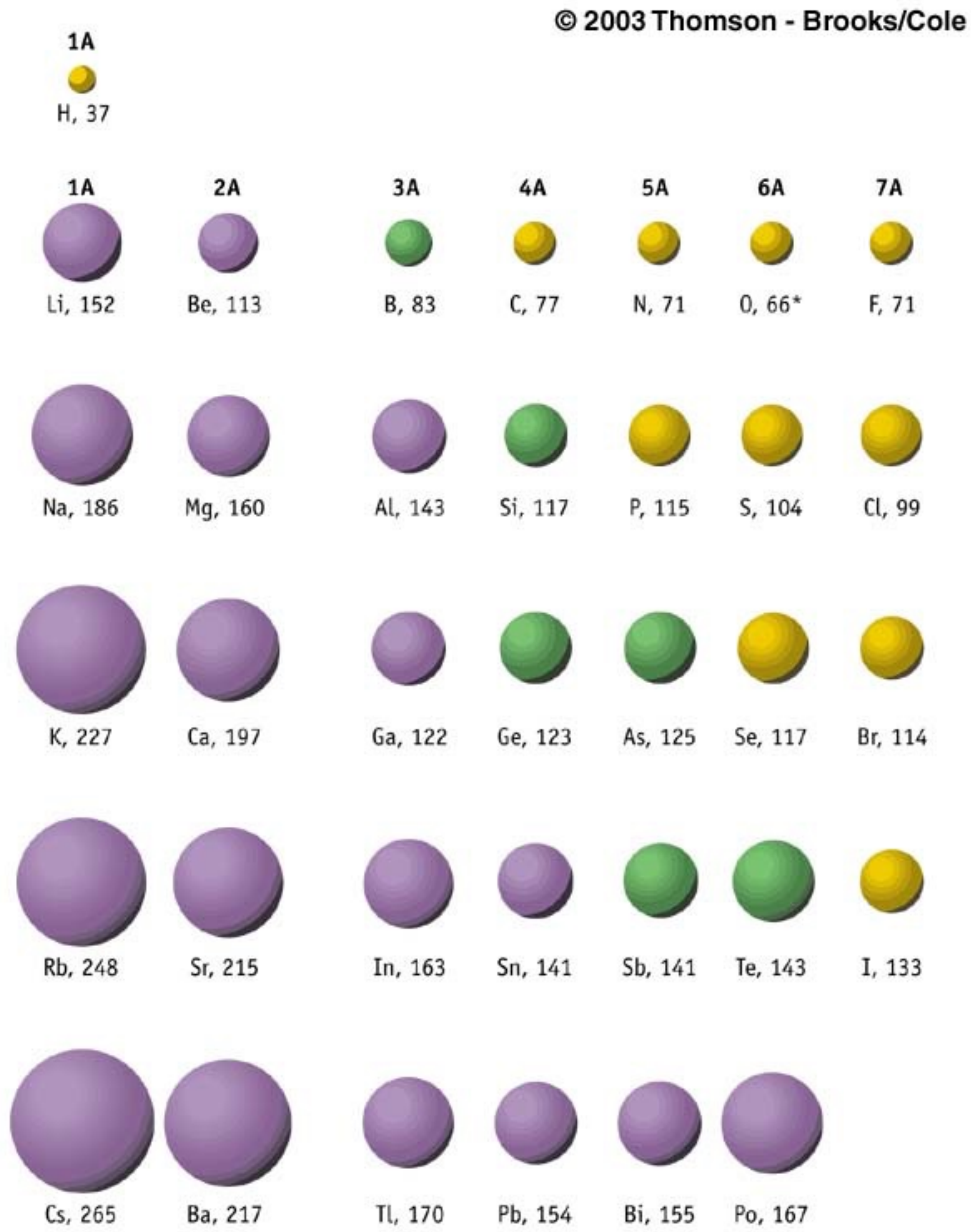
$X^+ + e^- \rightarrow X$

For most of the atoms and for all the positive ions the addition of an electron results in a release of energy ($\Delta E<0$).

The electron affinity is generally more negative toward the right along a period (except for noble gases) and upwards within a group.



Periodicity of electron affinity



Periodicity of the atomic radii for the main groups.

Periodicity of the properties of elements