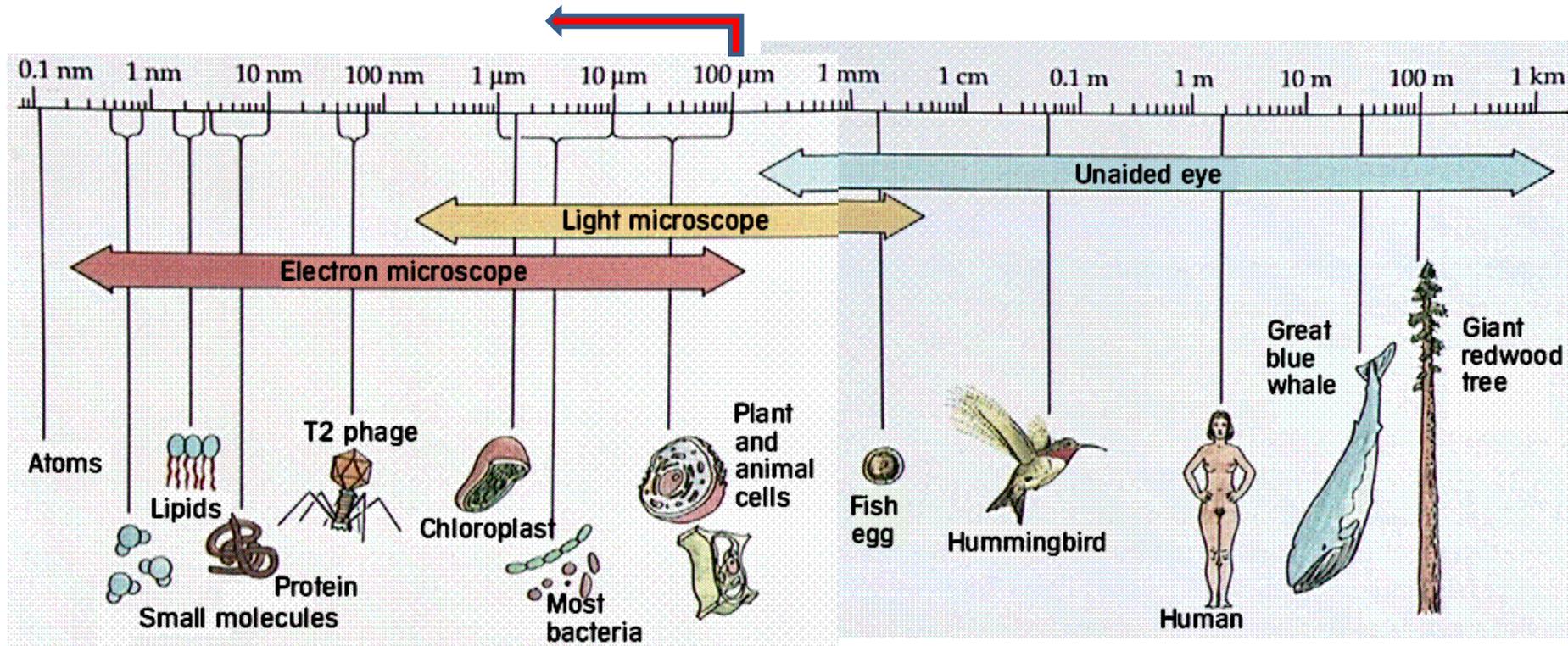


# Chemical introduction

Katalin Kiss, Gergely Berta

# SIZE-SCALE

Metric = in meter/in metre



Millimeter= mm    1 mm=10<sup>-3</sup>m

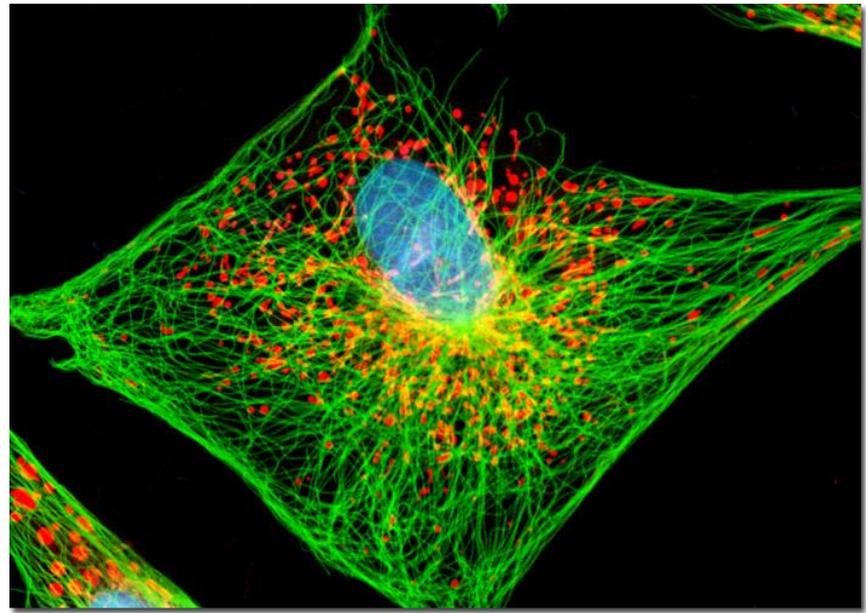
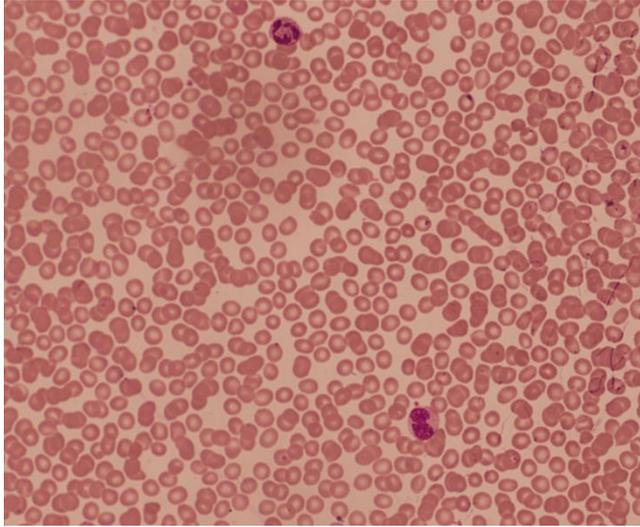
Mikrometer=μm    1 μm=10<sup>-6</sup>m

Nanometer=nm    1 nm=10<sup>-9</sup>m

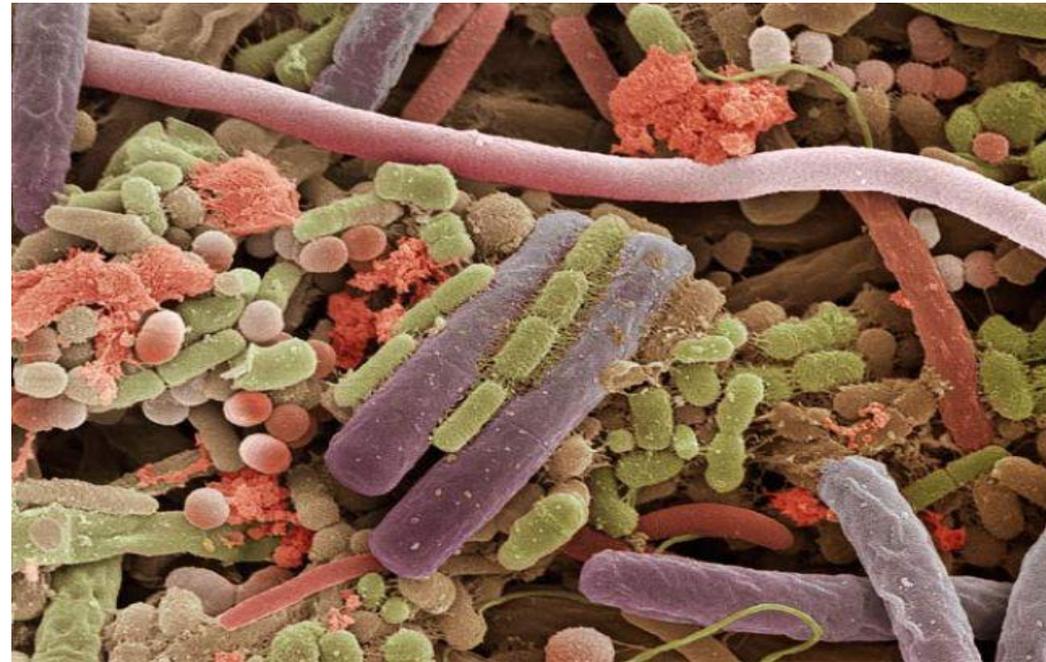
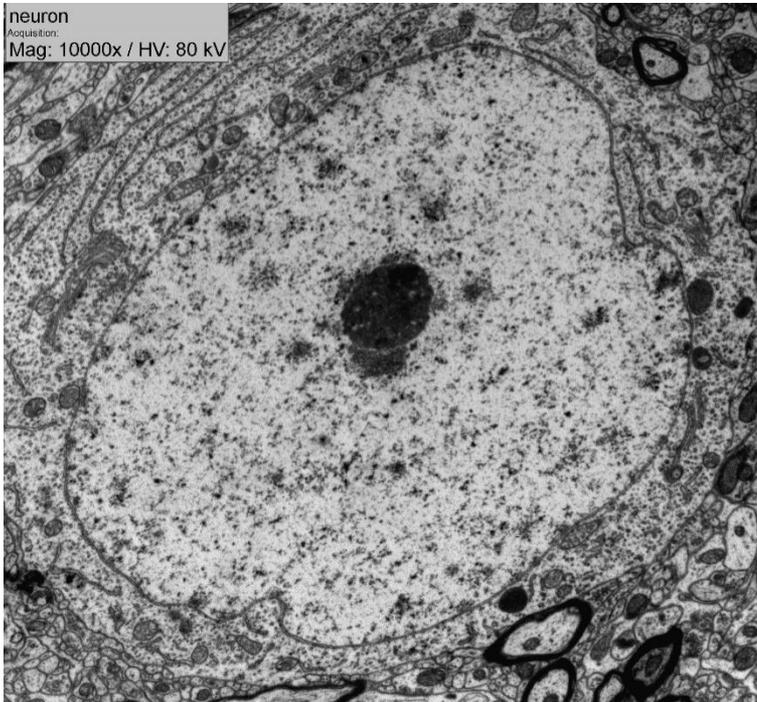
Centimeter=cm    1 cm=10<sup>-2</sup>m

Kilometer=km    1 km=10<sup>3</sup>m

- Light microscopy



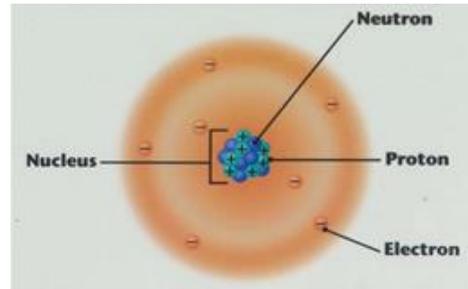
- Electron microscopy



# atom, ion, isotope, element, molecule

1. A substance composed of atoms with the same atomic number; it cannot be broken down in ordinary chemical reactions.
2. The smallest indivisible particle of matter that can have an independent existence.
3. Two or more atoms which are chemically combined to form a single species.
4. An atom that has lost or gained electrons from its outer shell and therefore has a positive or negative charge, respectively; symbolized by a superscript plus or minus sign and sometimes a number, e.g.,  $\text{H}^+$ ,  $\text{Na}^+$ ,  $\text{O}^{2-}$ ,  $\text{Cl}^-$ .
5. Atoms with the same atomic number but different numbers of neutrons; indicated by adding the mass number to the element's name, e.g., carbon 12 or  $^{12}\text{C}$ .

# Atom, subatomic particles



[www.csmate.colostate.edu](http://www.csmate.colostate.edu)

- **2 parts of an atom: nucleus** and electron **cloud** („1cm/100m”)
- Electron **orbital**: space of one electron
- Electron **shells**
  - composed of orbitals
  - determine the size of the atom
  - 4 major shells (K: 2 electrons, L: 8 electrons, M: 18 electrons, N: 32 electrons)
- Number of protons=number of electrons
- Atom is neutral=uncharged
- **Atomic number**: number of protons
- **Atomic mass/weight = mass number**: number of protons + number of neutrons

# Subatomic particles

Name	Charge	Location	Mass	Atomic mass
Proton	+1	atomic nucleus	$1.6726 \times 10^{-27}$ kg	1Dalton
Neutron	0	atomic nucleus	$1.6750 \times 10^{-27}$ kg	1Dalton
Electron	-1	electron orbital	$9.1095 \times 10^{-31}$ kg	negligible (1/1800Da)

Dalton = Da = unit of mass/weight (NOT METRIC!)

1 Dalton = mass/weight of 1 Hydrogen ion (H<sup>+</sup>)

1 Dalton = mass/weight of 1/12 Carbon atom

Mass/weight of proteins, eg. 60 000Da=60kDa

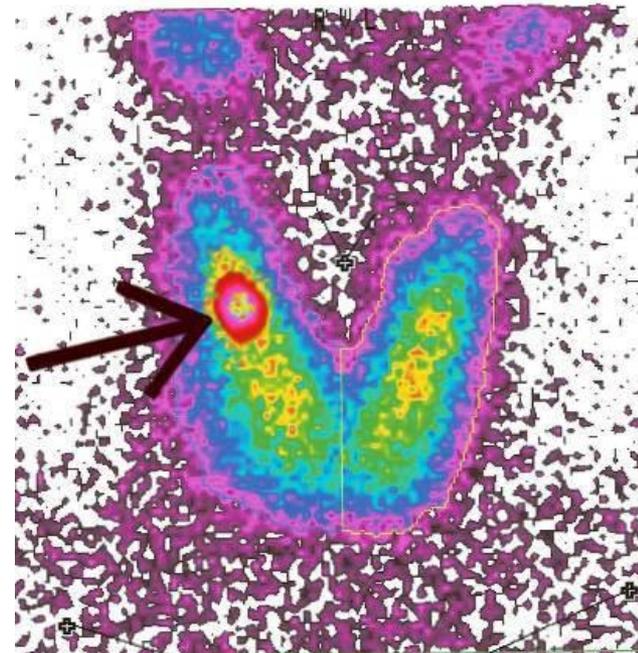
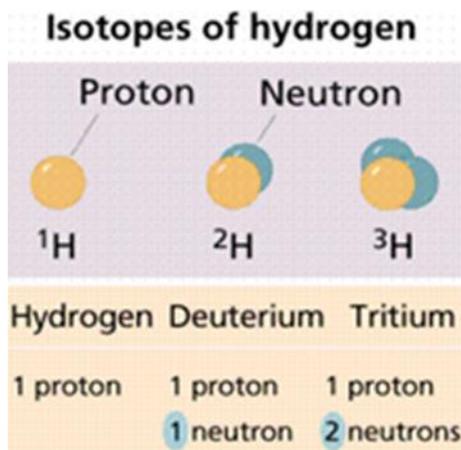
Kilodalton (kDa)=  $10^3$  Dalton

# Ions

- **more or less electrons than protons**
- charged
- types:
  - cation** (+ charge) : 1<sup>st</sup> and 2<sup>nd</sup> groups tend to lose 1 or 2 electrons  
eg. Na<sup>+</sup>, Mg<sup>2+</sup>
  - anion** (- charge) : 6<sup>th</sup> and 7<sup>th</sup> groups tend to gain 2 or 1 electrons  
eg. Cl<sup>-</sup>, O<sup>2-</sup>
- ionic bond formation

# Isotopes

- Same number of protons but different number of neutrons = **Same atomic number** but **different mass number**
- Types: stable and unstable (radioactive=nuclear splitting, fission)
- Types of radiation (particles emitted during fission):
  - $\alpha$ : He nucleus (2 protons+ 2 neutrons)
  - $\beta$ : electron
  - $\gamma$ : photon (electromagnetic)
- Role in medicine and research: to trace molecules eg. radioactive iodine



# Periodic table

- **D. I. Mendeleev**
- **symbols of elements** (element: a substance composed of atoms with the same atomic number) carbon:C; nitrogen: N; calcium: Ca etc.
- rows=**periods**: elements with the same major quantum number/same major electron shell (K, L, M, N)
- columns=**groups**: elements with the same versatile/unpaired electrons
- **Size of elements** increases from top to bottom and from right to left.
- **electronegativity**  
The different elements have a different attraction towards electrons.  
Electron affinity of elements increases from bottom to top, and from left to right.  
The highest electronegativity is possessed by fluorine (F).
- **relative atomic mass = molar mass** : gram/mole , mole: $6 \times 10^{23}$

# Atoms, subatomic particles, ions, isotopes III.

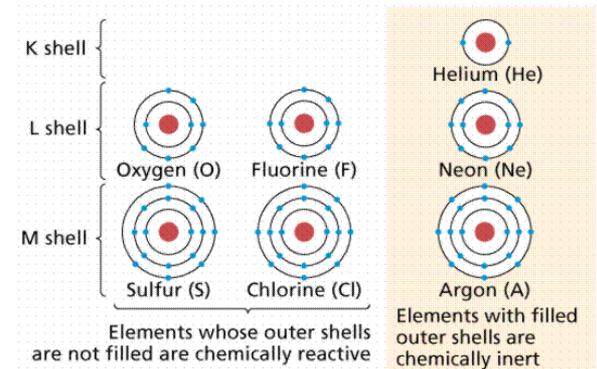
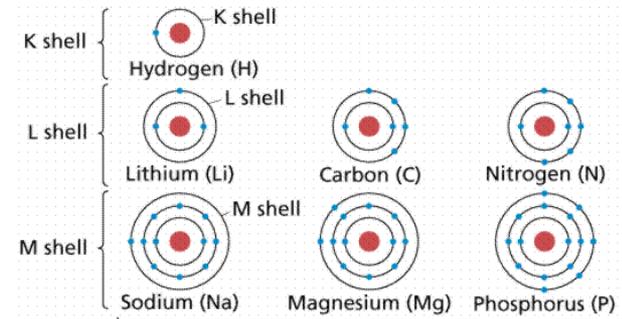
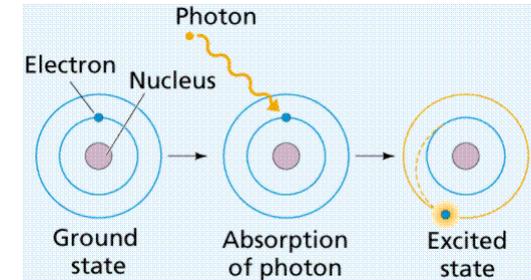
**Prof Mokeur's Periodic Table**

**Legend**

- Alkali Metals (Yellow)
- Alkaline Earth Metals (Light Blue)
- Transition Metals (Dark Blue)
- Metals (Green)
- Metalloids (Purple)
- Nonmetals (Light Green)
- Halogenes (Orange)
- Noble Gases (Light Yellow)
- Lanthanides and actinides (Grey)

**Hydrogen (H) Data:**

- Symbol: H
- Atomic number: 1
- Relative atomic mass: 1.00794
- Electronegativity: 2.1
- Oxidation number: +1
- Name: Hydrogen

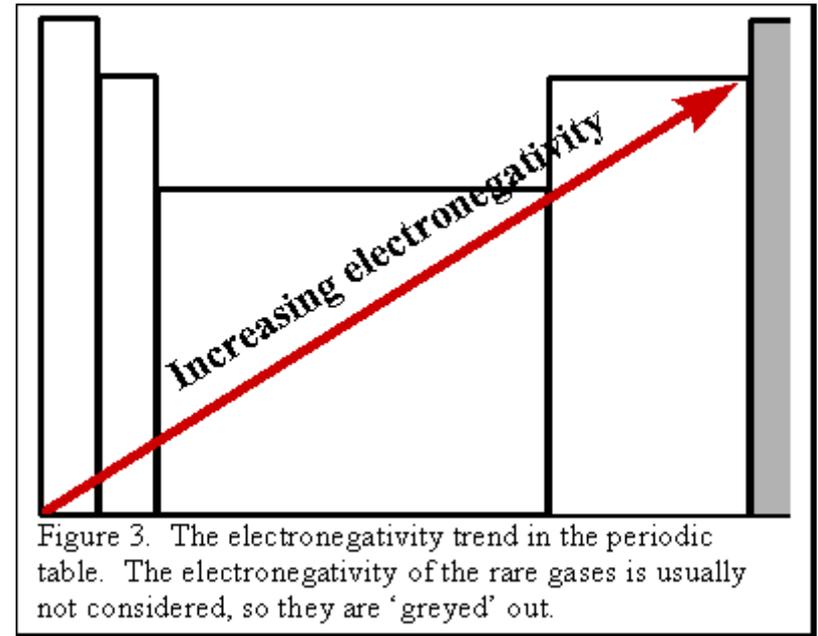
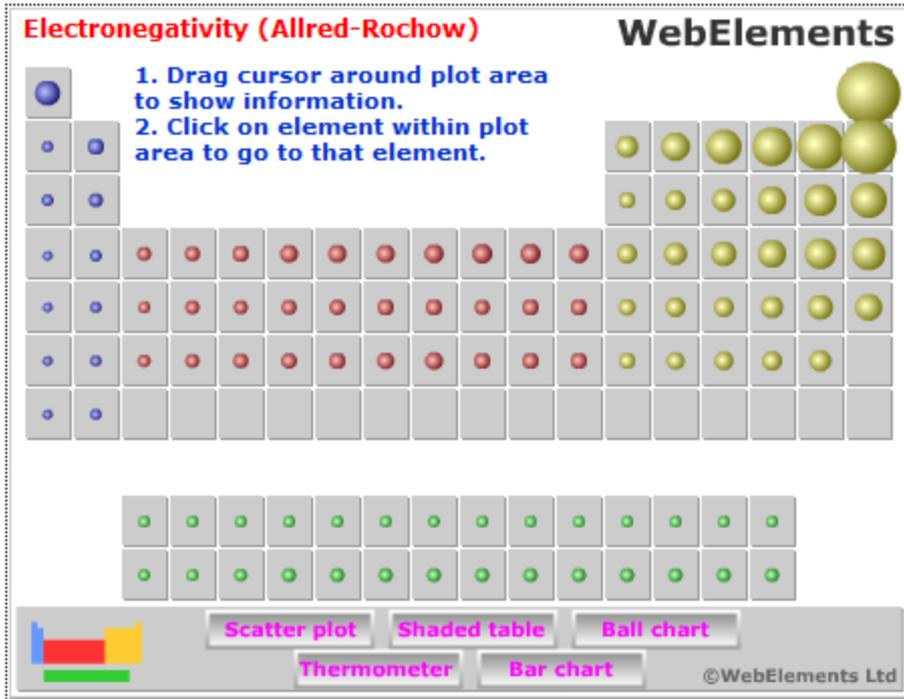


Lanthanides	6	<b>Ce 58</b> 140.116 1.1 3+	<b>Pr 59</b> 140.90765 1.1 3+	<b>Nd 60</b> 144.242 1.1 3+	<b>Pm 61</b> 144.9127 1.1 3+	<b>Sm 62</b> 150.36 1.2 3+	<b>Eu 63</b> 151.964 1.2 3+	<b>Gd 64</b> 157.25 1.2 3+	<b>Tb 65</b> 158.92535 1.2 3+	<b>Dy 66</b> 162.500 1.2 3+	<b>Ho 67</b> 164.93032 1.2 3+	<b>Er 68</b> 167.259 1.2 3+	<b>Tm 69</b> 168.93421 1.2 3+	<b>Yb 70</b> 173.03800 1.1 3+	<b>Lu 71</b> 174.967 1.2 3+
	Actinides	7	<b>Th 90</b> 232.0381 1.3 4+	<b>Pa 91</b> 231.03688 1.5 5+	<b>U 92</b> 238.02891 1.4 6+	<b>Np 93</b> 237.0482 1.3 5+	<b>Pu 94</b> 244.0942 1.3 4+	<b>Am 95</b> 243.0614 1.3 3+	<b>Cm 96</b> 247 1.3 3+	<b>Bk 97</b> 247.0703 1.3 3+	<b>Cf 98</b> 251.0790 1.3 3+	<b>Es 99</b> 252.03 1.3 -	<b>Fm 100</b> 257.0851 1.3 -	<b>Md 101</b> 258.01 1.3 -	<b>No 102</b> 259.1009 1.3 -

Atomic masses are measured relative to the carbon isotope <sup>12</sup>C (IUPAC - 2007).

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# Electronegativity



1. A chemical property which describes ing
    - the tendency of an atom or a functional group to attract electrons (or electron density) towards itself .
    - the tendency to form negative ions.
  2. An atom's electronegativity is affected by:
    - atomic number and the
    - distance that its valence electrons reside from the charged nucleus.
- The higher the associated electronegativity number, the more an element or compound attracts electrons towards it.

# Molecules

- 2 or more **atoms bound to each other** through covalent bond(s)
- **central atom**
- **stable** compound
- **shape** determined by electronpairs and the electron attraction by atomic nuclei  
eg. Linear (H-H, O-C-O), V-saped (H-O-H)
- **polarity** determined by the electronegativity of atomic nuclei  
apolar (eg. H-H) or polar (eg. H-Cl) molecules

# Chemical bonds in organic chemistry

## 1. Primary bonds:

### a) Covalent bond:

- Electrons are shared by the bound atoms (bonding electrons)
- Strong
- Inside molecules=intramolecular
- Types:
  - Single (H-H, C-C, H-O-H), Double (C=O, C=C), Triple (C≡C, N≡N)
  - Non polarized, polarized

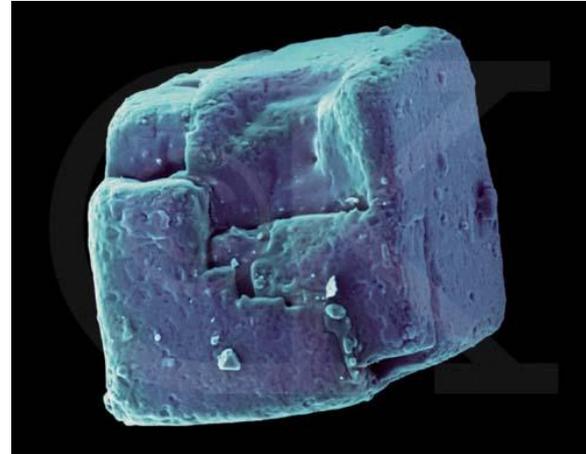
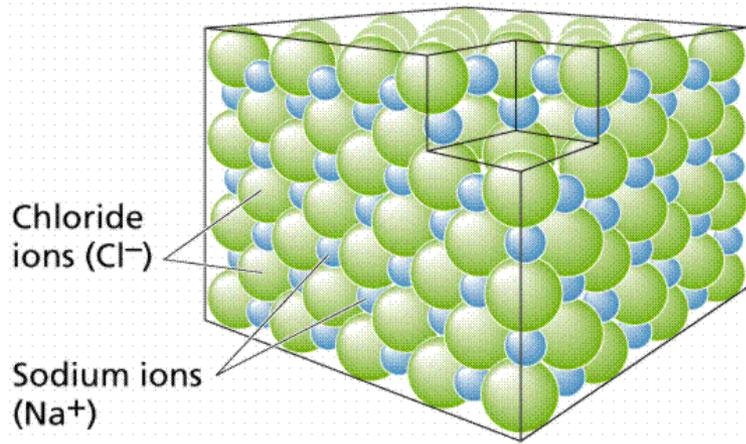
Disulfide-bond/Disulfide-bridge: -S-S- (inside molecules, between molecules)

### b) Ionic bond: between ions (eg. between Na<sup>+</sup> and Cl<sup>-</sup>)

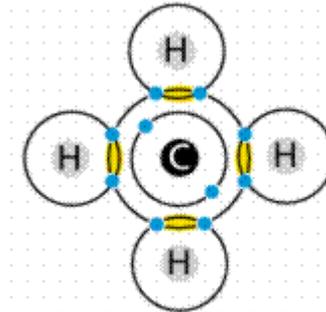
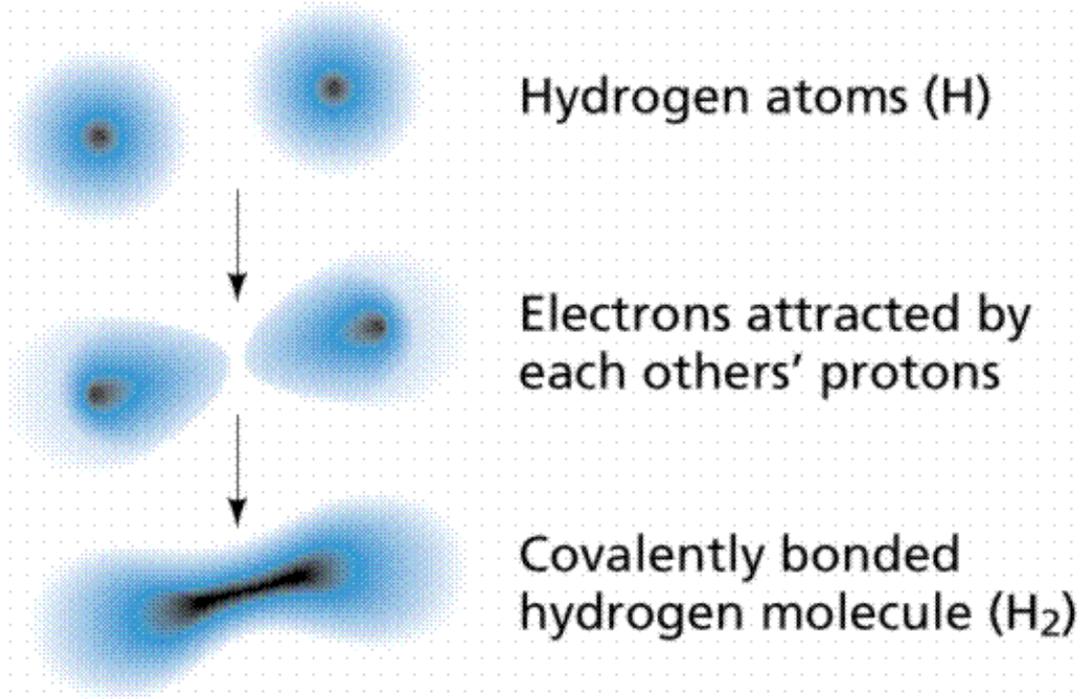
## 2. Secondary/Non-covalent bonds:

- electrons are not shared by the bound atoms
- Weaker than covalent bonds
- Between molecules =intermolecular
- Types:
  - Van der Waals=London forces (between apolar molecules)
  - Dipole-dipole bonds (between polar molecules)
  - Hydrogen bond

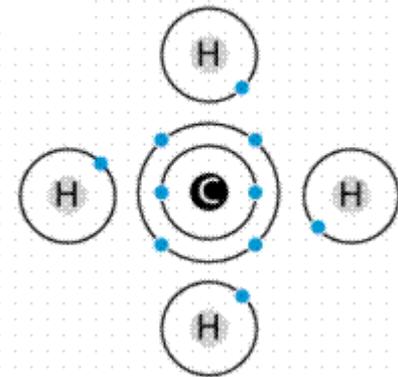
# Chemical bonds



# Chemical bonds

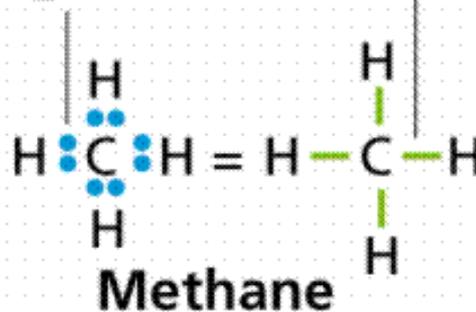


Methane

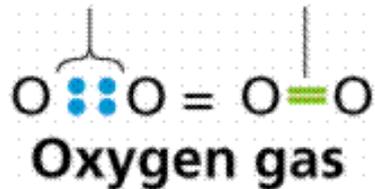


# Chemical bonds

Single covalent bond



Double bond

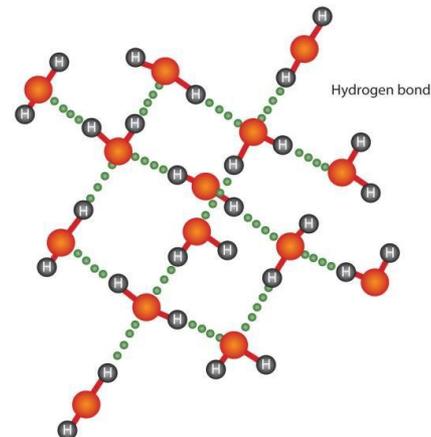


Triple bond

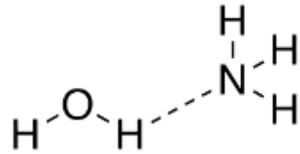


# Hydrogen bond

- is a secondary bond
- **between a H atom covalently attached to an electronegative atom** (atom with a high affinity for electrons) eg O, N, F **and an electronegative atom of another molecule or another part of the same molecule**
- weaker than covalent bonds
- between water molecules, inside protein molecules

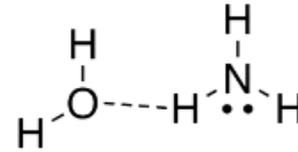


# Chemical bonds



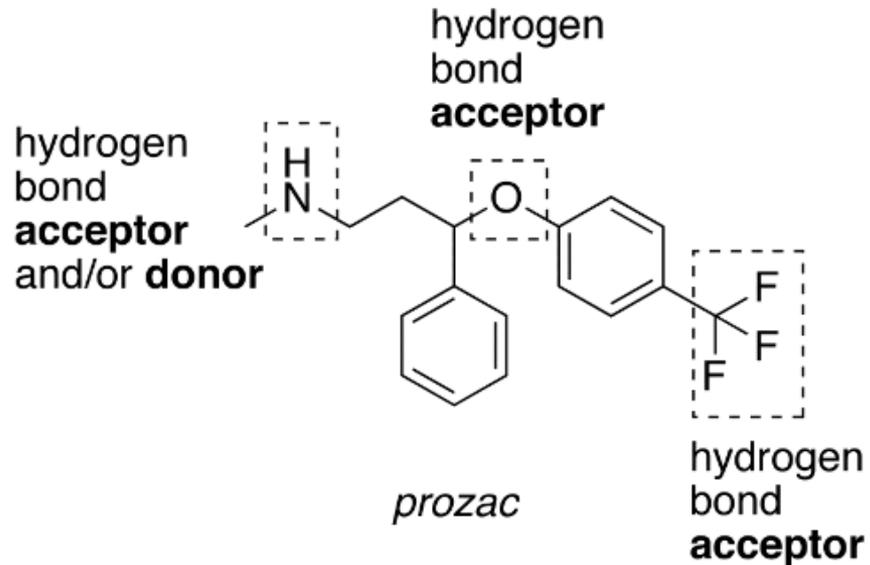
hydrogen  
bond  
**donor**

hydrogen  
bond  
**acceptor**



hydrogen  
bond  
**acceptor**

hydrogen  
bond  
**donor**



# Functional groups / chemical groups in organic chemistry

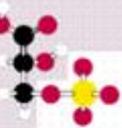
A complex of covalently joined atoms (minimum 2 atoms are coupled to each other).

The group is covalently linked to the carbon backbone (skeleton) of a molecule.

The group is responsible for

- the chemical properties of the molecule (eg. solubility, polarity, charge, acidic/basic feature...)
  - eg. Soluble in water and polar solvents: hydrophilic
  - Soluble in apolar solvents: hydrophobic (lipophilic)
- the chemical interactions (bond forming capability) of the molecule.

# Functional groups in organic chemistry

Functional group	Class of compounds	Structural formula	Example	Ball-and-stick model	Water solubility	Acid/Base	Charge	Molecules	Bonds
Hydroxyl -OH	Alcohols	R-OH	$\begin{array}{c} \text{H} & \text{H} \\   &   \\ \text{H}-\text{C} & - & \text{C}-\text{OH} \\   &   \\ \text{H} & \text{H} \end{array}$ Ethanol		yes	no	no	carbohydrates	ester
Carbonyl -CHO	Aldehydes	R-C(=O)H	$\begin{array}{c} \text{H} & \text{O} \\   &    \\ \text{H}-\text{C} & - & \text{C}-\text{H} \\   & \\ \text{H} & \end{array}$ Acetaldehyde		yes	no	no	Carbohydrates eg. glucose	
Carbonyl -CO-	Ketones	R-C(=O)-R	$\begin{array}{c} \text{H} & \text{O} & \text{H} \\   &    &   \\ \text{H}-\text{C} & - & \text{C}-\text{C}-\text{H} \\   & &   \\ \text{H} & & \text{H} \end{array}$ Acetone		yes	no	no	Carbohydrates eg. fructose	
Carboxyl -COOH	Carboxylic acids	R-C(=O)OH	$\begin{array}{c} \text{H} & \text{O} \\   &    \\ \text{H}-\text{C} & - & \text{C}-\text{OH} \\   & \\ \text{H} & \end{array}$ Acetic acid		yes	acids	-	Citric acid=citrate Aminoacids	ester peptide
Amino -NH <sub>2</sub>	Amines	R-NH <sub>2</sub>	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{N}-\text{H} \\   \\ \text{H} \end{array}$ Methylamine		yes	bases	+	aminoacids	peptide
Phosphate -OPO <sub>3</sub> <sup>2-</sup>	Organic phosphates	R-O-P(=O)(O <sup>-</sup> ) <sub>2</sub>	$\begin{array}{c} \text{HO} & \text{O} \\ \diagdown & / \\ \text{C} & \\   & \\ \text{H}-\text{C}-\text{OH} & \text{O} \\   &    \\ \text{H}-\text{C}-\text{O}-\text{P}-\text{O}^- \\   & \\ \text{H} & \text{O}^- \end{array}$ 3-Phosphoglyceric acid		yes	acids	-	Nucleotides Nucleic acids Phospholipids	Ester Phospho- anhydride (macroerg)
Sulfhydryl -SH	Thiols	R-SH	$\begin{array}{c} \text{H} & \text{H} \\   &   \\ \text{H}-\text{C} & - & \text{C}-\text{SH} \\   &   \\ \text{H} & \text{H} \end{array}$ Mercaptoethanol		yes	no	no	Aminoacids eg. cysteine	disulfide

# Biogenic elements

- elements present in living systems
- appr. 25
- types:
  - primary
  - secondary
  - tertiary =trace

1. „I bring forth acid”

2. **oxygen**

From Greek "όξύ γείνομαι" (oxy geinomai), which means "I bring forth acid", as it was believed to be an essential component of acids.

3. „I form water”

**Carbon** From the French, "charbons", which in turn came from Latin "carbō", which means "charcoal" and is related to "carbōn-", which means "a coal".

4. **I form native-soda**

**Hydrogen** From French hydrogène[28] and Latin hydro- and -genes, derived from the Greek, "ύδωρ γείνομαι" (hydor geinomai), meaning "I beget water".

6. **light bearer**

**Nitrogen** From French "nitrogène",[38] derived from Greek "νίτρον γείνομαι" (nitron geinomai), meaning "I form/beget native-soda (nitrate)".

7. **pot-ash**

8. **salicyllow**

**Calcium** From Latin "calx", which means "lime". Calcium was known as early as the first century when the Ancient Romans prepared lime as calcium oxide.

9. **soda**

**Phosphorus** From Greek φῶς + -φόρος (phos + -phoros), which means "light bearer", because "white phosphorus" emits a faint glow upon exposure to oxygen. "Phosphorus" was the ancient name for "Venus", or Hesperus, the (Morning Star).[18]

11. **violet**

**Potassium** From the English "potash", which means "pot-ash" (Potassium compound prepared from an alkali extracted in a pot from the ash of burnt wood or tree leaves). The symbol K is from Latin name, Kalium, from Arabic ("القلي al qaliy), which means "calcined ashes".

12. **strong metal, holy metal**

**Sulfur** Almost certainly from Arabic ("صفرأ sufra), "yellow", the bright color of the naturally occurring form.

13. **yellowish green/ greenish yellow**

**Sodium** From the English, "soda" used in names for Sodium compounds such as caustic soda, soda ash, and baking soda. The symbol Na is from modern Latin noun natrium, derived from Greek "νίτρον" (níttron), "natural soda, a kind of salt" + Latin -ium.[

14. **Moon**

**Magnesium** From the Ancient Greek, "Μαγνήσια" (Magnesia) (district in Thessaly), where discovered.

15. **flint (a kind of stone)**

**Iodine** Named after the Greek, "ιώδης" (iodes), which means "violet", because of the color of the gas. This word was adapted as the French iode, which is the source of the English iodine

16. **bitter salt**

**Iron** meaning "holy metal" or "strong metal" which in its turn may derive from the Etruscan, aisar, meaning "the god(s)", because the earliest iron to be worked was obtained from meteorites, and meteorites fall from the sky.[31]The symbol Fe is from Latin ferrum, meaning "iron".

**Chlorine** From Greek "χλωρός" (chlorós), which means "yellowish green" or "greenish yellow", because of the color of the gas.

**Selenium** From Greek, "σελήνη" (selene), which means "Moon", and also moon-goddess Selene

**Silicon** From Latin "silex" or "silicis", which means "flint", a kind of stone.

**Aluminium** Latin alumen, which means "alum" (literally "bitter salt").

# Elements of human body

primary, secondary, tertiary (trace)

1. Oxygen (65%)
2. Carbon (18%)
3. Hydrogen (10%)
4. Nitrogen (3%)
5. Calcium (1.5%)
6. Phosphorus (1.0%)
7. Kalium/Potassium (0.35%)
8. Sulfur (0.25%)
9. Natrium/Sodium (0.15%)
10. Magnesium (0.05%)
11. Copper, Zinc, Selenium, Molybdenum, Fluorine, Chlorine, Iodine, Manganese, Cobalt, Iron (0.70%)
12. Lithium, Strontium, Aluminum, Silicon, Lead, Vanadium, Arsenic, Bromine ( $\leq 0,5\%$ )

Essential trace elements:

-are elements present in small quantities in living cells, organisms but vital for cells

# Elements of human body

**oxygen:** 2 valence electrons, electronegative

- in water
- in CO<sub>2</sub>
- in all organic molecules, in many functional groups
- in H-bond formation
- oxygenates H into water during ATP (energy) synthesis  
= oxidant

**carbon:** 4 valence electrons

- formation of carbon backbone=skeleton of organic molecules (central atom)
  - formation of complex and diverse molecules
  - formation of single, double, triple bonds
  - formation of linear, and ring-like backbones
- in many functional groups
- in CO<sub>2</sub>
- is oxidized during breakdown processes (eg. glucose breakdown)

**hydrogen:** 1 valence electron

- in water
- in all organic molecules, in many functional groups
- in H-bond formation
- is reduced into water during ATP (energy) synthesis

# Elements of human body

**nitrogen:** 3 valence electrons, electronegative

- in aminoacids and proteins
- in nucleotides and nucleic acids (purine, pyrimidine bases)
- (in a few lipids, carbohydrates)
- in amino group
- in H-bond formation

**calcium:**

- bones, teeth (rigidity)
- blood coagulation
- muscle contraction

**phosphorous:**

- bones, teeth (rigidity)
- in nucleotide, nucleic acids
- in phosphate functional group

# Elements of human body

## **sodium=potassium and calcium=calcium:**

- membrane potential, action potential

## **sulfur:**

- in thiol functional group
- in aminoacids, proteins

## **magnesium:**

- in enzyme function
- in muscle cell and nervous system function

## **iodine:**

- in thyroid gland hormone (thyroxine)

## **iron:**

- in haemoglobin (O<sub>2</sub> gas transport in blood)