Astrobiology
Lecture 3

Water & carbon in terrestrial life

SISSA, Academic Year 2023
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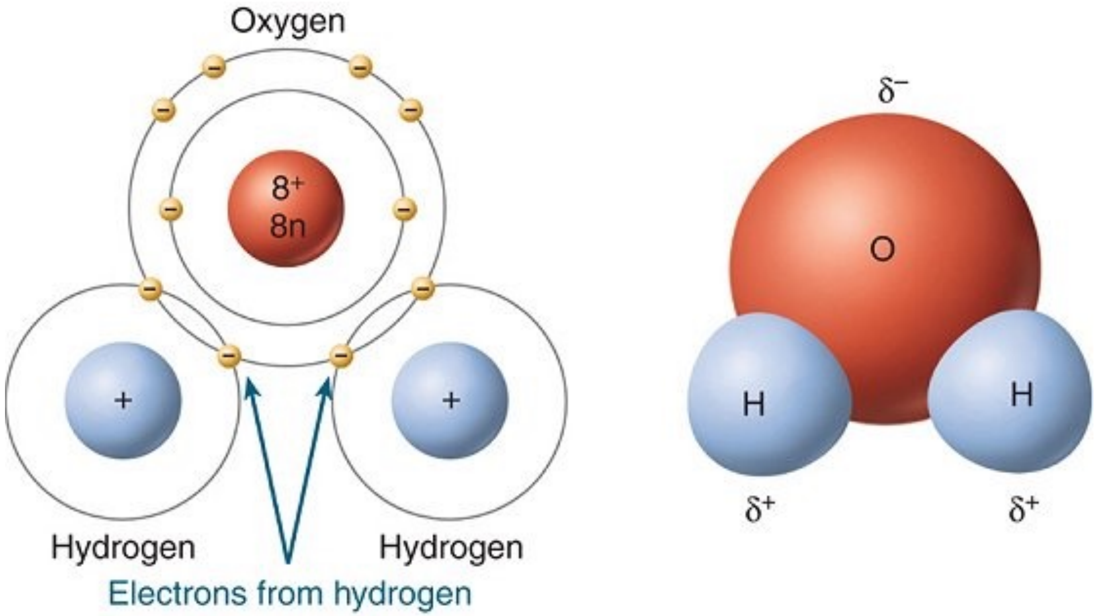
The water molecule

Builds up the molecular medium of terrestrial life

The water molecule is polar



(a) Electron shells in a water molecule

(b) Distribution of partial charges in a water molecule

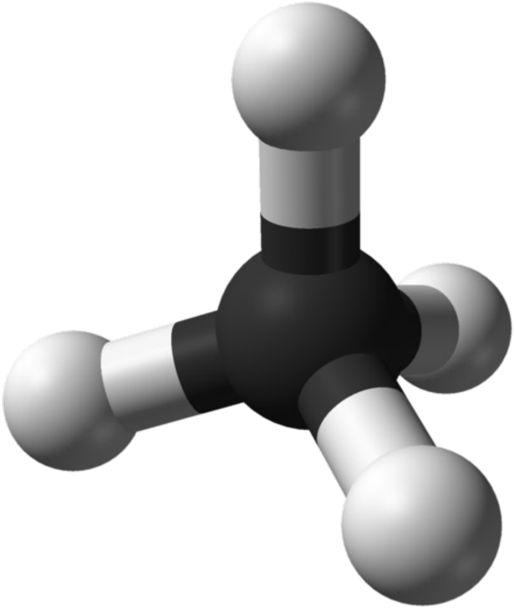
Polar and non-polar molecules

- The polar character depends on the geometrical distribution of electric charges of the molecule

  Water is polar because of the asymmetric distribution of charges

  Methane is non polar (no electric dipole)

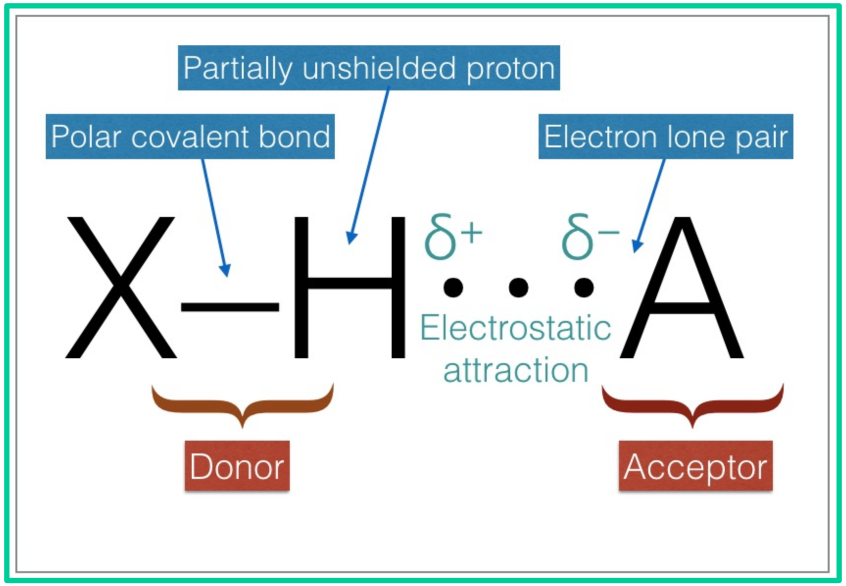
Methane:
a non-polar molecule

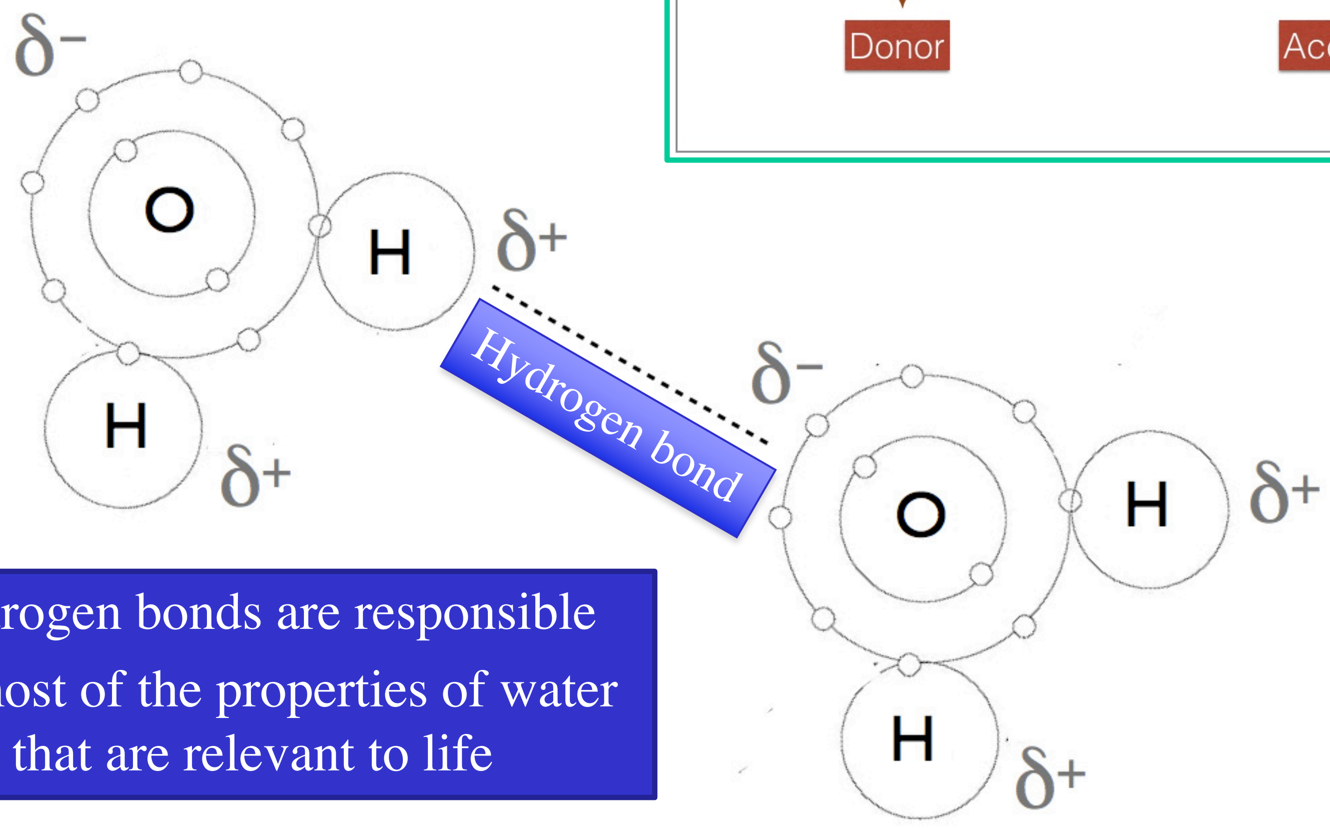


- Polar molecules
  - can be solved in water
  - are hydrophilic

- Non-polar molecules
  - cannot be solved in water
  - are hydrophobic

Water molecules are connected by a network of hydrogen bonds





Hydrogen bonds are responsible for most of the properties of water that are relevant to life

Properties of water relevant to life (1)

- The water molecule has a high electric dipole
  - Water is a good solvent

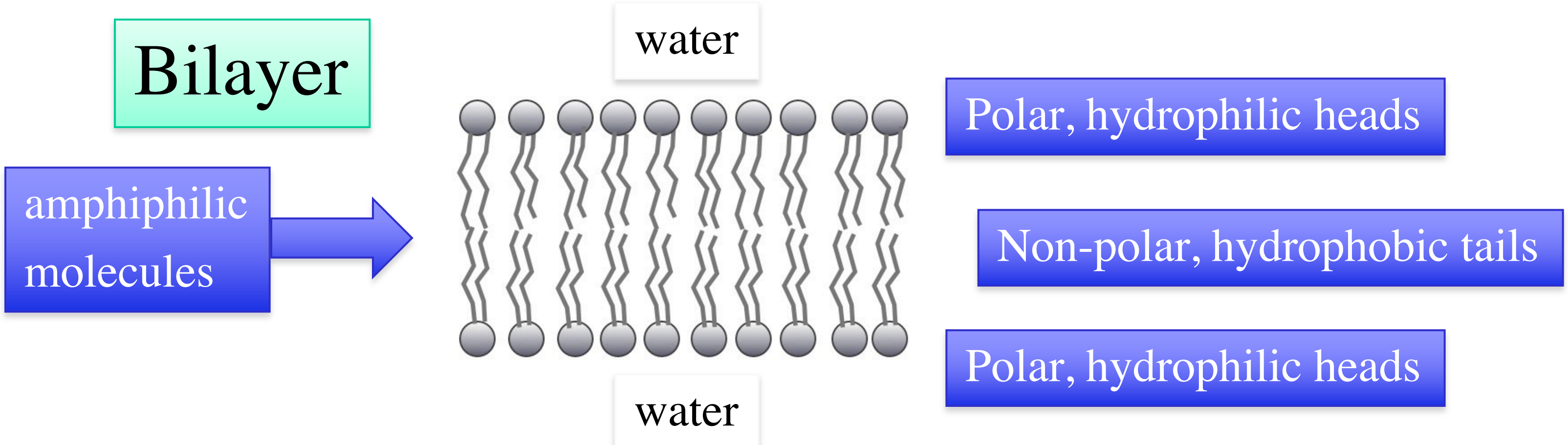
    Thanks to this property, life molecular constituents can be dissolved and have the mobility required for metabolic processes to take place

    Biomolecules also take advantage of the external structural support provided by water molecules

  - Thanks to the polarity, amphiphilic molecules in water can spontaneously form structures of biological interest (bilayers, micelles)

    Amphiphilic molecules: two-ended molecules with one end hydrophilic and one end hydrophobic

Polar molecules allow spontaneous formation of molecular structures of biological interest



The spontaneous formation is driven by entropy variations

Although the clustering results in a decrease of entropy of the dissolved molecules, fewer water molecules are required to encase the clustered structures and a larger number of water molecules are free to move (net entropy increase)

Atkins & De Paula, Physical Chemistry for Life Sciences, 2011, p. 86

Properties of water relevant to life (2)

- Water spontaneously form ions
  - Spontaneous breaking of covalent bonds in a small fraction of water molecules yields H^+ and OH^- ions

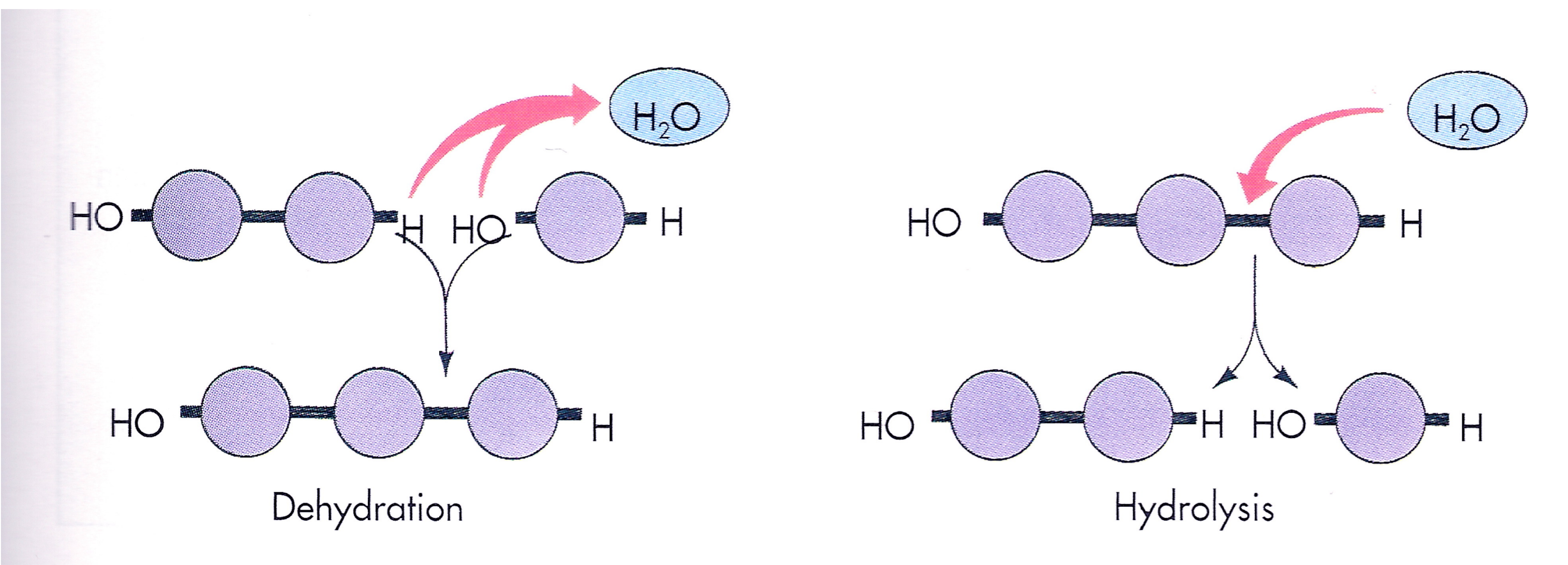
Note: the concentration of H^+ ions in water is used to define the pH scale

The free ions, and in particular H^+,
can be used to transport electric charges

H^+ and OH^- take part in metabolic reactions

- Water takes part of fundamental metabolic processes, both as a <u>reactant</u> and as a <u>product of reaction</u>

- Water formation and dissociation plays a direct role in metabolic processes



Carbon in terrestrial life

Electronic orbitals

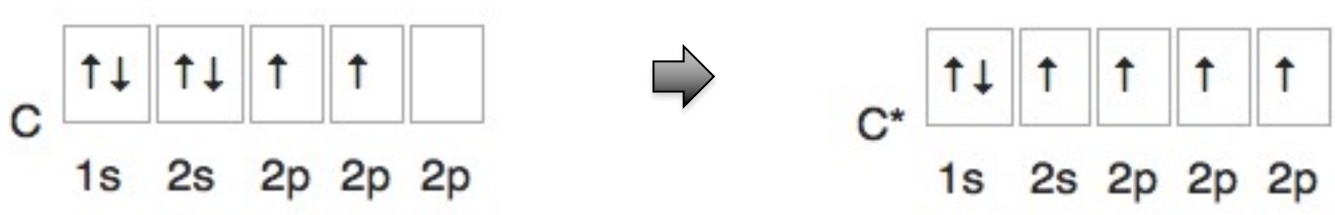
Carbon-based biological macro-molecules

Carbon

In terrestrial life carbon is the building block of biological molecules

- With respect to other cosmically abundant atoms, carbon offers several advantages in terms of structural and metabolic properties

- Electronic configuration
  - Carbon's ground state configuration is $1s^2\ 2s^2\ 2p^2$

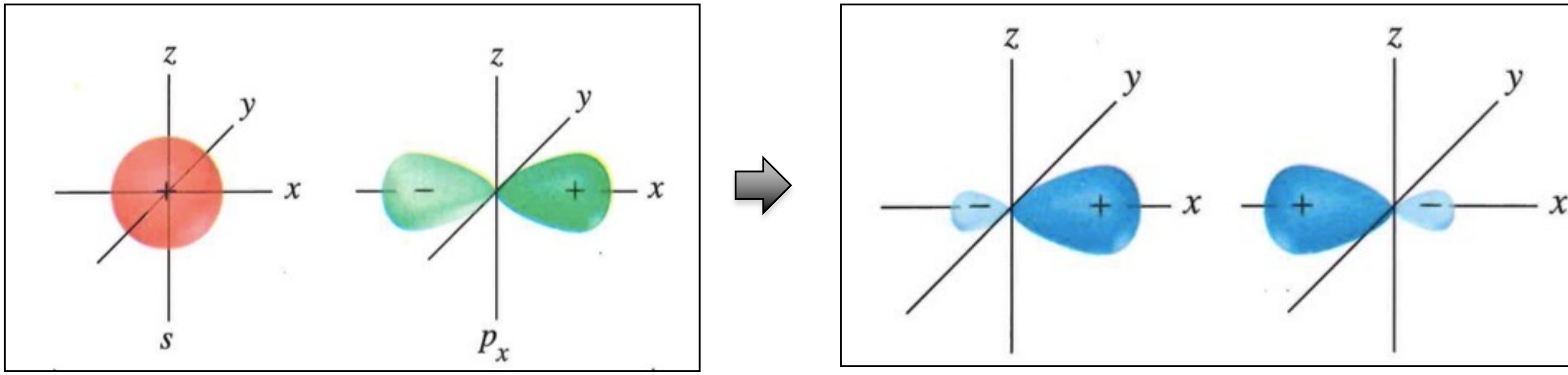


  - The excitation of one electron of the 2s orbital easily provides a configuration with 4 orbitals with a single electron
  - The 4 oriented covalent bonds allow the formation of a great variety of 3D molecular structures:

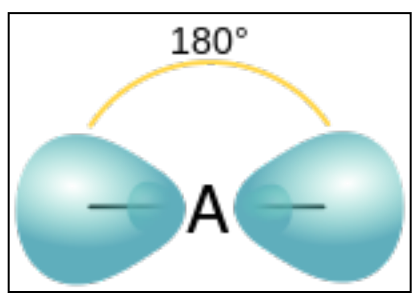
linear, planar, tetrahedical

Hybridization of carbon valence orbitals

sp orbitals: two atomic orbitals are mixed to form two hybrid orbitals

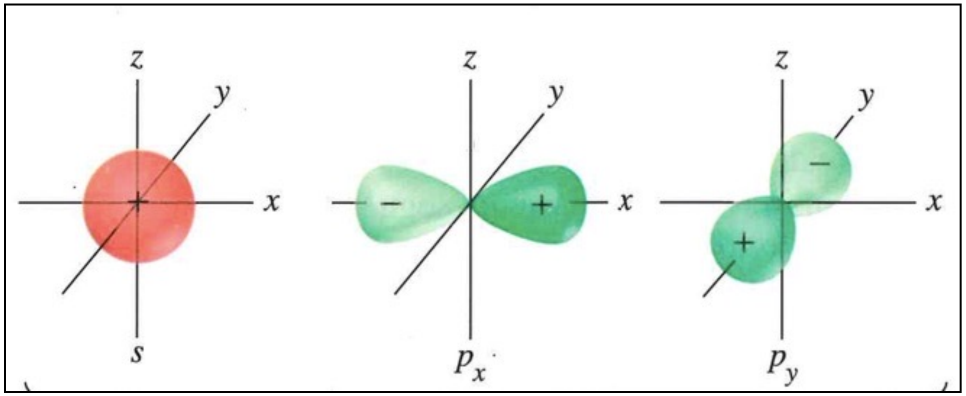


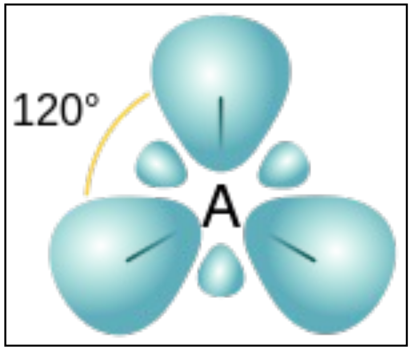
The two sp hybrid orbitals arrange themselves in three dimensional space to get as far apart as possible with a bond angle of 180°.
The geometry which achieves is linear.



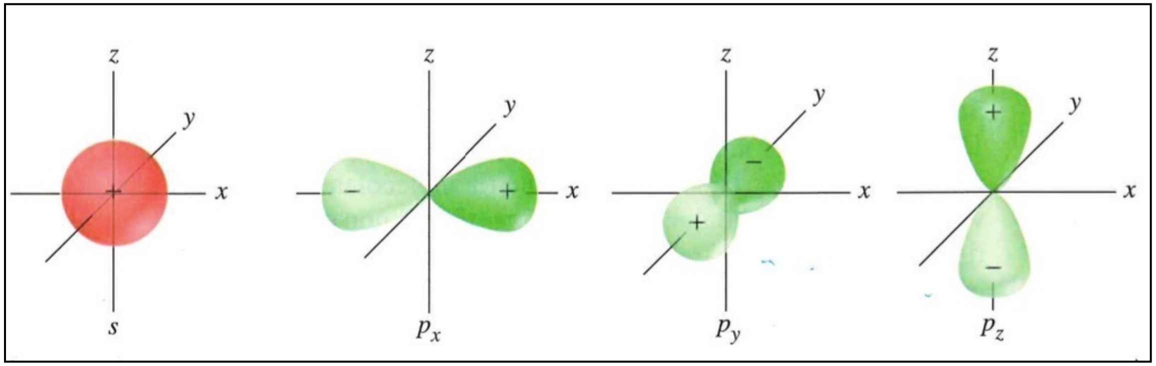
Hybridization of carbon valence orbitals

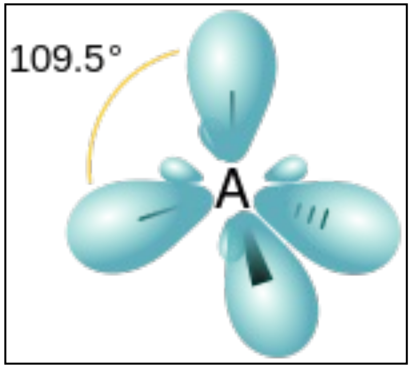
sp² orbitals: three atomic orbitals are mixed to form three hybrid orbitals





sp³ orbitals: four atomic orbitals are mixed to form four hybrid orbitals





Carbon

- Structural properties
  - In summary, carbon has 4 oriented covalent bonds that allow the formation of a great variety of 3D molecular structures

  - The valence orbitals 2s and 2p can hybridize forming:

    two sp hybrid orbitals ➔ linear structures

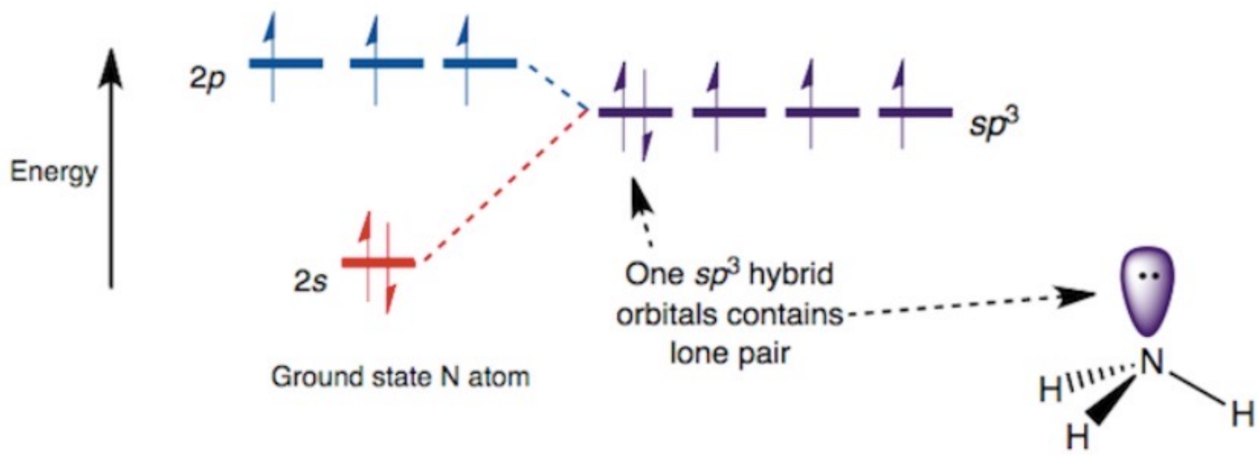
    three sp^2 hybrid orbitals ➔ planar structures

    four sp^3 hybrid orbitals ➔ tetrahedrical structures

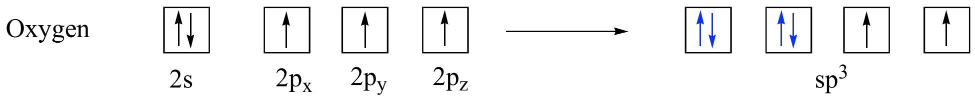
Carbon versus nitrogen and oxygen

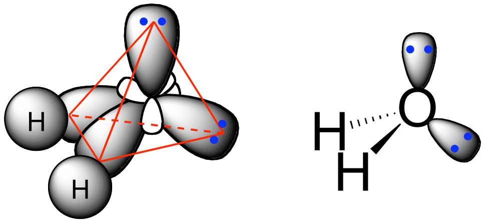
The flexibility of carbon to form 3D structures is not found in other atoms

Nitrogen has 3 covalent bonds which tend to form planar structures



Oxygen has 2 covalent bonds which tend to form linear structures

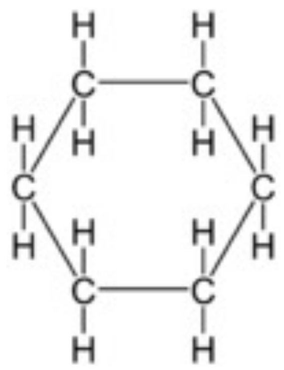




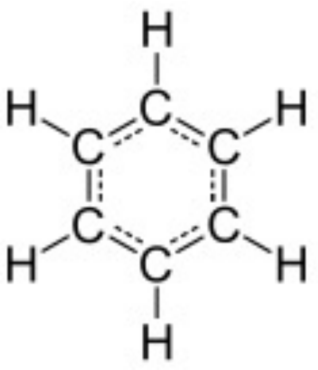
Organic ring structures

Carbon can form a variety of ring structures

Carbon is the only atom with the capability of forming aromatic rings



Cyclohexane
(saturated molecule)



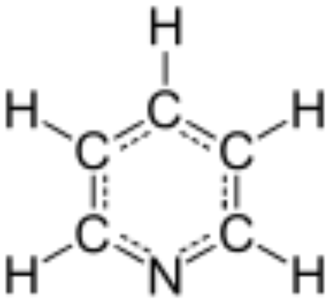
Aromatic ring of Benzene
(unsaturated molecule)

Hetero-organic molecules

- Carbon is capable of forming complex molecules not only with itself, but also with H, O and N

  This is because the covalent bonds C-C, C-H, C-O, and C-N have similar dissociation energies

  For instance, N can replace C in ring structures



The large flexibility of carbon in terms of geometrical structure, coupled with the possibility of substitutions of other abundant elements, leads to a infinite number of possible molecular structures (organic chemistry)

The huge spectrum of molecular structures offered by organic chemistry is particularly important in biochemistry

Advantages of carbon

Metabolic properties

- Carbon can easily be transformed from the completely oxidized form, CO_2, to the completely reduced form, CH_4

This is an advantage for the capability of activating metabolic processes, which are largely based on redox reactions

Redox: reducing-oxidating reactions

This property provides the possibility of cycling carbon between its "inorganic form" and its "organic form"

CO_2 : inorganic carbon

CH_4 : organic carbon

The great capability of carbon to form complex structures is supported by astronomical observations of interstellar molecules

All interstellar molecules with at least 6 atoms are organic

Table 5.4 Some complex carbon compounds detected in the interstellar medium and meteorites.

Number of Atoms				
6	7	8	9	> 9
C_5H, HCH_2OH	CH_3C_2H	CH_3OCHO	$(CH_3)_2O$	$(CH_3)_2CO$
NH_2CHO,	CH_3CHO	CH_3C_3N	CH_3CH_2OH	HC_9N
CH_3CN	HC_5N, C_6H	C_7H, H_2C_6	CH_3CH_2CN	$HC_{11}N$
CH_3NC,	CH_3NH_2		HC_7N	C_6H_6, $C_{60}{}^+$
CH_3SH	CH_2CHCN		CH_3C_4H, C_8H	PAHs,
H_2C_4,	C_2H_4O		CH_3C_4N	glycine?
HCC_2HO,				
C_5H, C_5N,				
C_5O				

From carbon atoms to biological macromolecules

Carbon is the most abundant constituent
of the macromolecules of terrestrial life

Biological macromolecules

The most important biomolecules of terrestrial life are macromolecules with a large number of atomic units (e.g., $10^6 – 10^8$ amu)

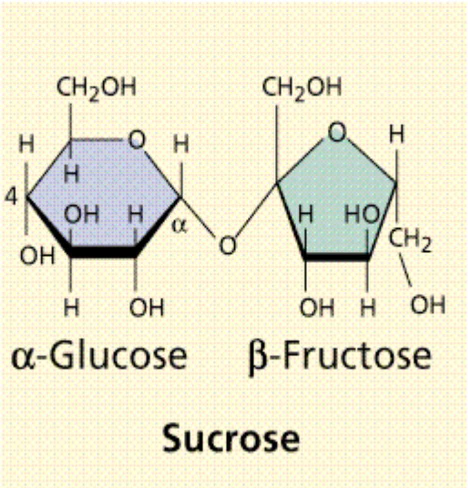
Macromolecules result from the polymerization of a large number of subunits (monomers)

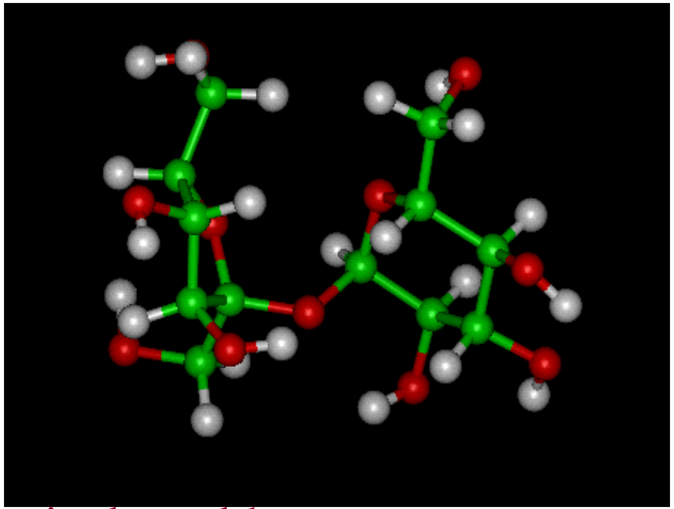
Terrestrial life features 4 types of macromolecules:

carbohydrates, lipids, proteins and nucleic acids

energy storage	compartmentalization	metabolic	genetic

Carbohydrates (saccharides)





The most abundant molecules in the biological world

Primary source of chemical energy for most organims

General formula: $C_x(H_2O)_y$

Monosaccharides (simple sugars)

Oligosaccharides

From 2 to 10 units of monosaccharides

Polysaccharides

More than 10 monosaccharides

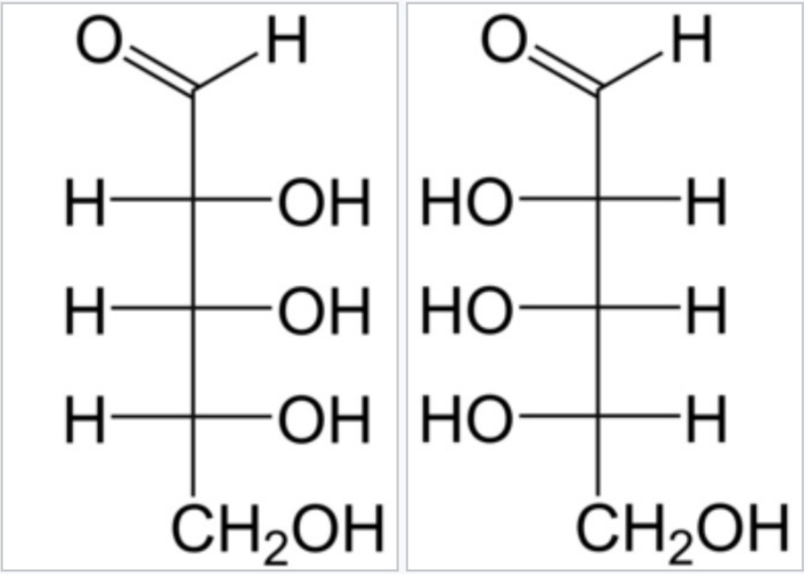
Carbohydrates

Ribose

Simple sugar that is found in RNA

In biology only appears in the form D-ribose

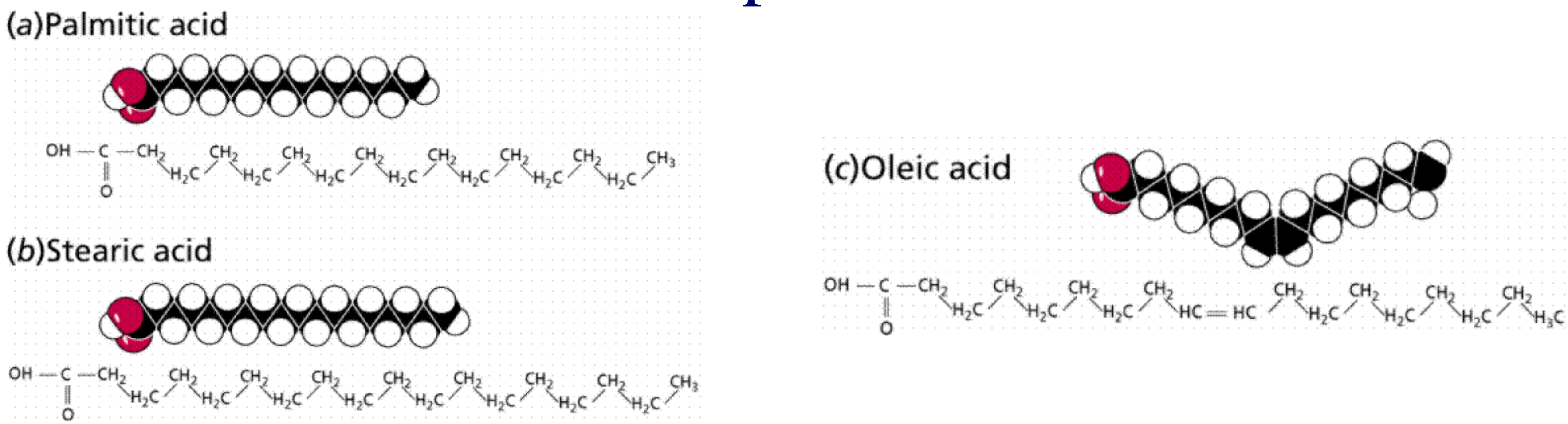
Example of homochirality of biological molecules



D-ribose L-ribose

Biological macromolecules

Lipids



Heterogeneous class of organic molecules with common solubility properties

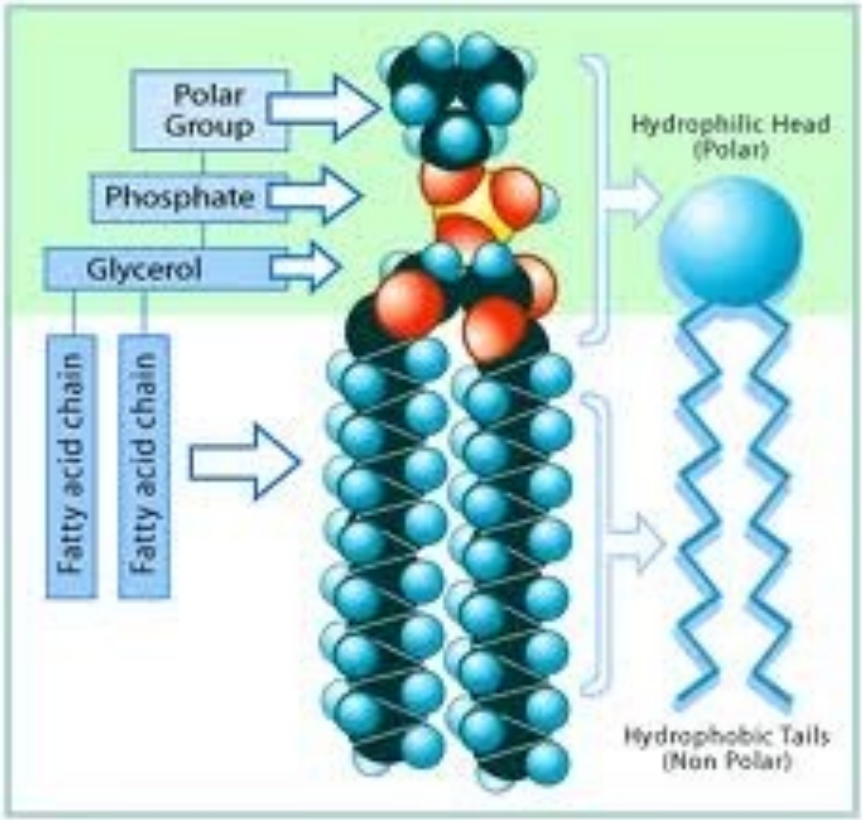
- Insoluble in water
- Soluble in certain types of non-polar solvents

Larger number of C–H bonds with respect to carbohydrates

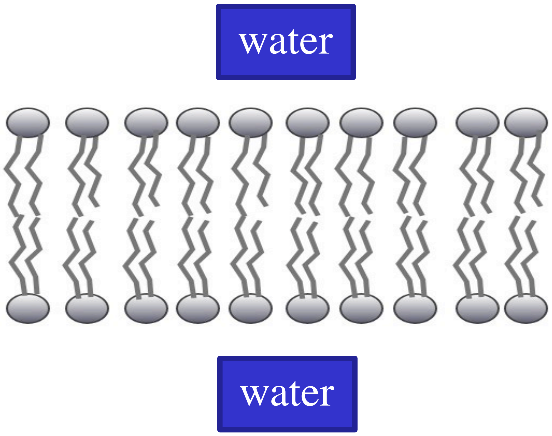
- Used for long-term storage of energy

Phospholipids

Examples of <u>amphiphilic</u> molecules with a <u>hydrophilic</u> end and a <u>hydrophobic</u> end



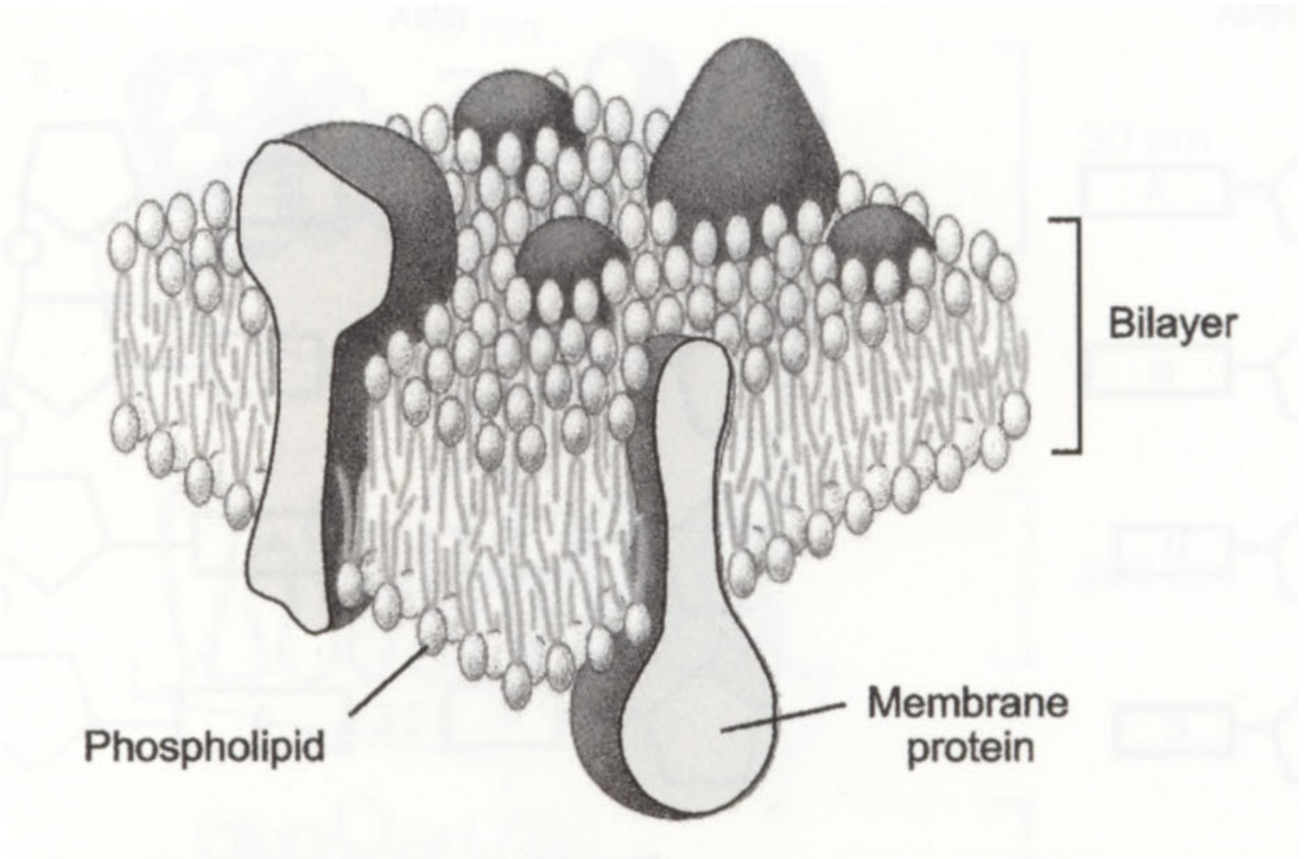
In liquid water phospholipids <u>spontaneously</u> form a double layer of molecules (<u>bilayer</u>), with the hydrophobic ends facing each other in the inner part, and the hydrophilic ends facing the water



Phospholipids and cell membranes

Bilayers of phospholipids are the main structural components of cell membranes

Specialized proteins embedded in the bilayer provide the possibility to exchange molecular constituents in and out of the cell

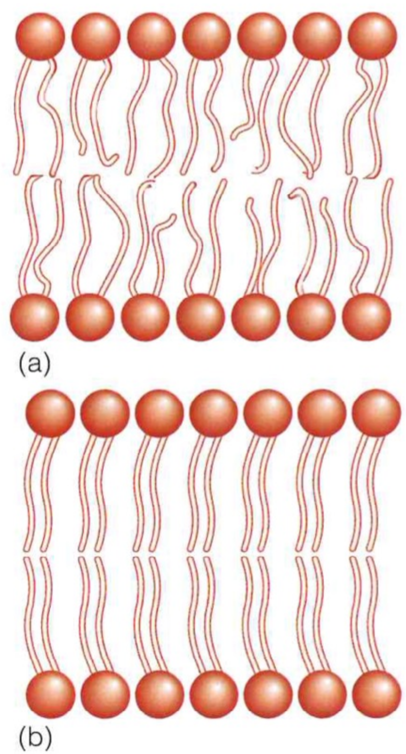


Phase transitions of biological membranes

Cell membranes need to be sufficiently rigid to encase life’s molecular machines while being flexible enough for cell division

Physiological temperature:
liquid crystal

Below a limiting temperature:
gel (frozen motion)



Atkins & De Paula, Physical Chemistry for Life Sciences, 2011, p. 108