EXPLORING MOLECULAR STRUCTURES USING AVOGADRO : BEYOND SIMPLE MOLECULES

Different classes of molecules to be investigated:

- Alkanes
- Alkenes
- Cyclic molecules
- Aromatics
- Isomers
- Amphiphiles
- Polymers

ALKANES

- Alkanes are compounds that consist only of carbon and hydrogen atoms with the general formula : $\mathbf{C_nH_{2n+2}}$
- The simplest alkane is **methane** (CH_4)

- Subsequent members of the series are:
  - Ethane (C_2H_6)
  - Propane (C_3H_8)
  - Butane (C_4H_{10}) … and so on.

- They are also referred to as saturated hydrocarbons (consist of only single bonds).
- Bond lengths are **1.09Å** for a C-H bond and **1.54Å** for a C-C bond.
- They are obtained as byproducts from the oil and natural gas industry.

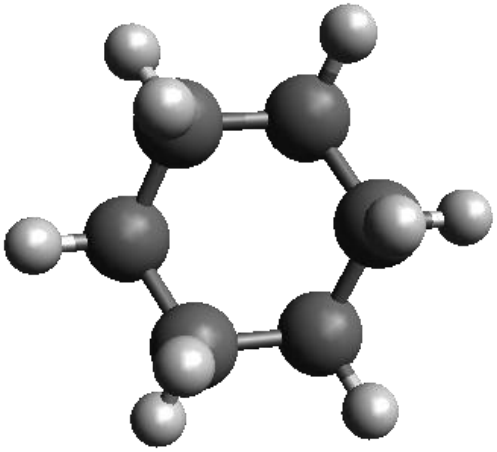
ALKENES

- Alkenes are chemical compounds that consist of at least one carbon-carbon double bond (unsaturated hydrocarbon).
- They form a homologous series with the general formula : $\mathbf{C_nH_{2n}}$
- The simplest alkene is **ethene** (C_2H_4)
- Subsequent members of the series are:
  - Propene (C_3H_6)
  - 1-Butene (C_4H_8)
  - 1-Pentene (C_5H_{10}) … and so on.

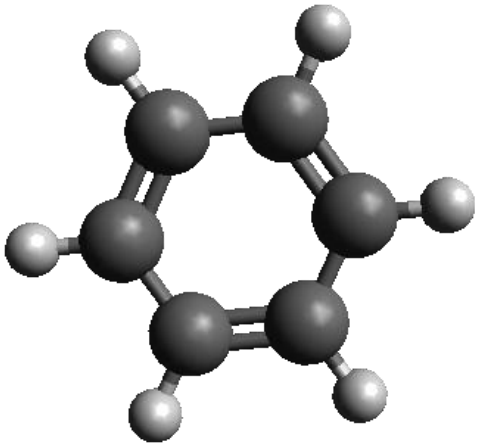
- Bond lengths are **1.09Å** for a C-H bond, **1.54Å** for a C-C single bond and **1.33Å** for a C=C double bond.
- The double bond is almost 1.75 times stronger than a single bond.

CYCLIC MOLECULES

- Cyclic compounds are those that have a series of atoms that are connected by bonds to form a ring.
- Alkanes and alkenes can also form cyclic structures. For example cyclopentane, cyclohexane, benzene, etc.
- Simple cyclic compounds have one ring structure whereas more complex ones can have many rings (polycyclic compounds).



Cyclohexane - chair/boat conformation



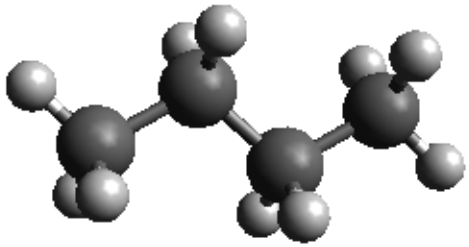
Benzene – Planar structure

AROMATIC COMPOUNDS

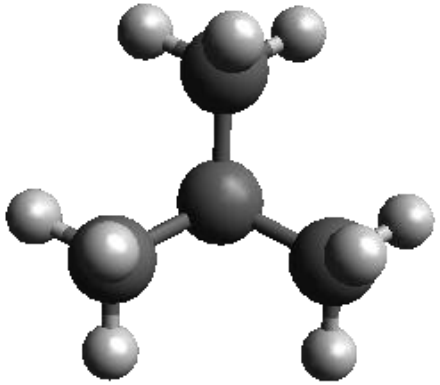
- Aromatic compounds have certain characteristic features:
  - They have a ring structure with an alternating single and double bond arrangement.
  - All atoms in the ring are present in the same plane.
- Aromatic compounds are widely present in our body. DNA, RNA and some essential amino acids are all made up of aromatic compounds.
- Industrially, aromatic compounds are used as raw materials in the manufacture of a wide variety of polymers such as polystyrene and nylon.

ISOMERS

- Isomers are compounds that have the same molecular formula but different structural formula.
- For example, butane is a hydrocarbon that belongs to the alkane family and has four carbon atoms.
- Based on the structural arrangement of these carbon atoms, it is either called n-butane or isobutane (also called methylpropane).



n-butane

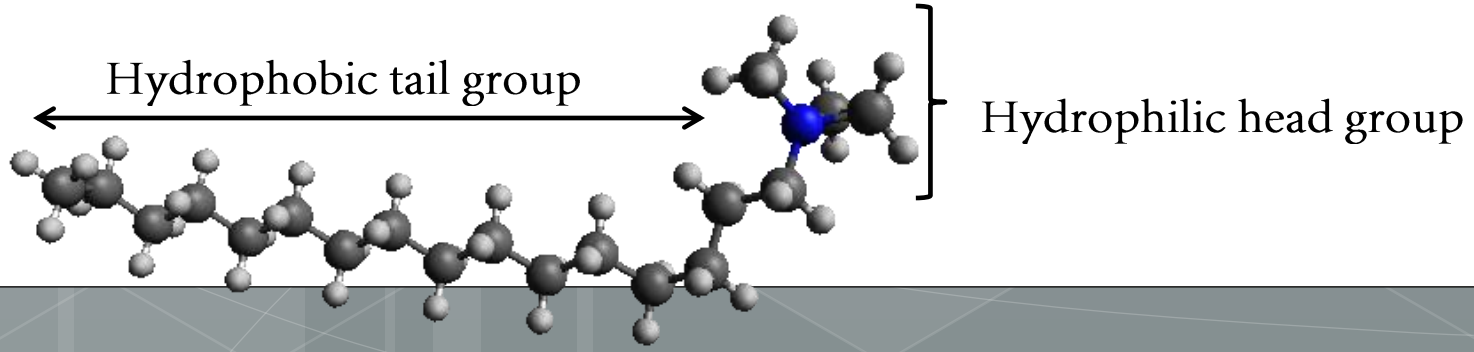


Isobutane

AMPHIPHILES

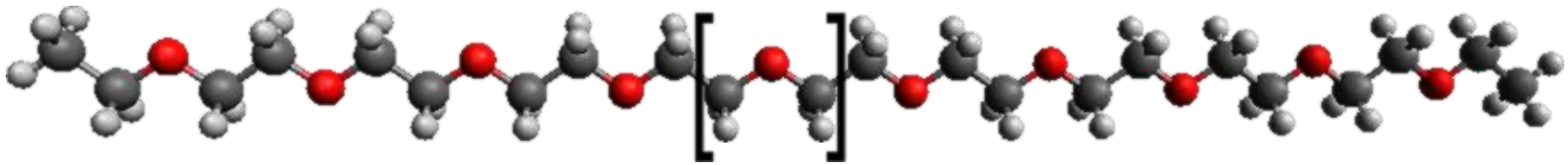
- Amphiphiles are molecules that have both hydrophilic (water-loving) and lipophilic (fat/oil-loving) groups.
- The hydrophobic part typically consists of a long hydrocarbon chain whereas the hydrophilic part can be either charged or polar.
- These molecules are most commonly found in soap, shampoo and detergents.

- Amphiphilic molecules that are commonly used in the manufacture of soaps and detergents are called SURFACTANTS (Surface Active Agents).
- The hydrophobic tails attach to the (oil-like) stain with the hydrophilic head groups projecting into the water.



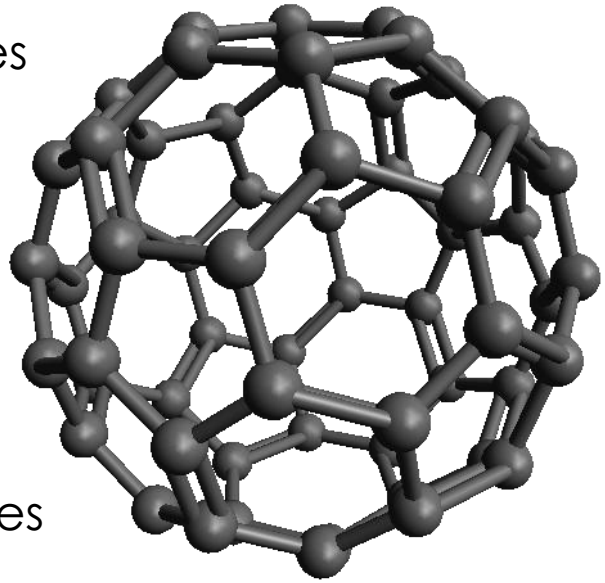
POLYMERS

- Polymers are large macromolecules that are made up of a number of repeating units called monomers.
- They are broadly classified into natural and synthetic polymers. Natural polymers include DNA, rubber and cellulose whereas synthetic polymers include polyethylene, polystyrene and nylon among many others.
- Polymers can possess a wide range of properties and are omnipresent.
- They prove to be of immense interest in the field of computational chemistry and biochemistry.



BUCKMINSTERFULLERENE

- Commonly referred to as buckyballs
- Discovered in 1985 by Robert Curl, Harold Kroto and Richard Smalley.
- Belong to a class of molecules called fullerenes
- Each carbon atom is bonded to 3 other carbon atoms
- It is a polygon with 60 vertices and 32 faces
- Extremely stable at high temperatures and pressures
- Readily reacts with anionic / electron rich species
- Can trap and protect atoms and molecules that are otherwise unstable.



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