What is Organic Chemistry?

- Based around the chemistry of **carbon**
  - and a few other elements (mainly H)

- Chemistry of **Life**
  - (proteins, nucleic acids, sugars.....)

- Involves:
  - transformations (**reactivity**)
  - and formation (**synthesis**) of organic structures
What is Organic Chemistry?

The Unique Nature of Carbon

- Carbon has atomic number = 6
- Electronic configuration: 1\text{s}^2 \ 2\text{s}^2 \ 2\text{p}^2
- Valence of 4 - four bonds to completely fill outer electron shell of carbon

Carbon can bond to:

- Itself - single, double, triple bonds
- Metals - eg Na, K, Fe, Cu, Mg ...
- Heteroatoms - eg N, P, O, S, F, Cl....

C-C and C-H bonds are strong:

\[
\begin{align*}
\text{C-C} & \approx 348 \text{ kJ mol}^{-1} \\
\text{C-H} & \approx 413 \text{ kJ mol}^{-1}
\end{align*}
\]

C-C and C-H bonds are non-polar.

A combination of the strength and non-polar nature make C-C and C-H bonds unreactive.

Can make rings, chains, multiple bonds (double or triple bonds);

tetravalence of C is satisfied by appropriate combination of single, double, triple bonds
What is Organic Chemistry?

Carbons unique bonding capabilities lead to:

- Structural complexity
- Molecular diversity

⇒ role in biology and industry

(chemistry of living organisms, medicines, dyes, polymers, food additives, pesticides......)
### Drawing Organic Structures

Most organic compounds have a *three dimensional* structure. How do we represent structures on our two-dimensional page?

For example methane is a tetrahedral molecule.

<table>
<thead>
<tr>
<th>Type</th>
<th>Hybridisation</th>
<th>Shape</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td><img src="image" alt="Example" /></td>
</tr>
</tbody>
</table>

- Bonds in the plane of the paper: C—H
- Bonds coming towards the observer: C→H
- Bonds going away from the observer: C||H
Drawing Organic Structures

Organic compounds may be represented in several ways:

Condensed structures:
Atoms are shown, bonds are understood
Atoms bonded to a C atom are listed after it.

Stick Representation:

- **Lines represent bonds**: 1 line for single bonds
  2 lines for double bonds \ multiple bonds
  3 lines for triple bonds /

- **Carbon atoms are not shown.** They are assumed to be present at the intersection of two or more bonds and at the end of each line.
- **Hydrogen atoms bonded to carbon are not shown.** They are assumed from the valence.
- **All heteroatoms are shown (+ H’s bound to heteroatoms)**
- **Remember when drawing neutral organic compounds:**

  - C has a valence of 4 (4 bonds, no lone pairs)
  - N has a valence of 3 (3 bonds, 1 lone pair)
  - O has a valence of 2 (2 bonds, 2 lone pairs)
  - X (halogens = F, Cl, Br, I) have a valence of 1 (1 bond, 3 lone pairs)

<table>
<thead>
<tr>
<th>Structural Formula Showing all Atoms &amp; Bonds</th>
<th>Stick Abbreviation</th>
<th>Condensed Structural Formula</th>
</tr>
</thead>
</table>
| \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{O} \\
\text{H} \\
\text{H} \\
\end{array}
\] | \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{O} \\
\text{H} \\
\text{O} \\
\text{H} \\
\text{O} \\
\text{H} \\
\end{array}
\] | CH₃CH₂COOH |
| \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\end{array}
\] | \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{O} \\
\text{H} \\
\text{O} \\
\text{O} \\
\text{O} \\
\end{array}
\] | CH₃CH₂COCH₃ |
| \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{Cl} \\
\text{H} \\
\end{array}
\] | \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{O} \\
\text{O} \\
\text{O} \\
\text{O} \\
\text{Cl} \\
\text{H} \\
\end{array}
\] | CH₃CH₂ClCH=CH₃ |
| \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\text{C} \\
\end{array}
\] | \[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{O} \\
\text{O} \\
\text{O} \\
\text{O} \\
\text{Cl} \\
\text{H} \\
\end{array}
\] | C₆H₅CN |
An organic compound can be viewed as a skeleton of carbon-carbon single bonds with "functional groups" attached at different positions.

- **Functional groups** are the *reactive parts* of an organic compound = multiple bonds and bonds to heteroatoms.

- Functional groups confer the characteristic chemical and physical properties of the compounds that contain them.

- Functional groups undergo the same chemical reactions irrespective of the type of molecule that contains them.

- A molecule with several functional groups displays reactivity which is the sum of the reactions that each functional group undergoes.

 Functional Groups in Organic Chemistry

<table>
<thead>
<tr>
<th>Family Name</th>
<th>Functional group structure</th>
<th>Simple example</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alkene</td>
<td><img src="functional_group_structure_alkene.png" alt="Functional group structure" /></td>
<td><img src="simple_example_alkene.png" alt="Simple example" /></td>
</tr>
<tr>
<td>Alkyne</td>
<td><img src="functional_group_structure_alkyne.png" alt="Functional group structure" /></td>
<td><img src="simple_example_alkyne.png" alt="Simple example" /></td>
</tr>
<tr>
<td>Arene</td>
<td><img src="functional_group_structure_arene.png" alt="Functional group structure" /></td>
<td><img src="simple_example_arene.png" alt="Simple example" /></td>
</tr>
<tr>
<td>Alkyl halide</td>
<td><img src="functional_group_structure_alkyl_halide.png" alt="Functional group structure" /></td>
<td><img src="simple_example_alkyl_halide.png" alt="Simple example" /></td>
</tr>
<tr>
<td>Family Name</td>
<td>Functional group structure</td>
<td>Simple example</td>
</tr>
<tr>
<td>---------------------</td>
<td>----------------------------</td>
<td>----------------</td>
</tr>
<tr>
<td>Alcohol</td>
<td><img src="image" alt="Alcohol structure" /></td>
<td>CH₃OH</td>
</tr>
<tr>
<td>Thiol</td>
<td><img src="image" alt="Thiol structure" /></td>
<td>CH₃SH</td>
</tr>
<tr>
<td>Ether</td>
<td><img src="image" alt="Ether structure" /></td>
<td></td>
</tr>
<tr>
<td>Amine (primary)</td>
<td><img src="image" alt="Amine (primary) structure" /></td>
<td>NH₂</td>
</tr>
<tr>
<td>Aldehyde</td>
<td><img src="image" alt="Aldehyde structure" /></td>
<td>H</td>
</tr>
<tr>
<td>Ketone</td>
<td><img src="image" alt="Ketone structure" /></td>
<td></td>
</tr>
<tr>
<td>Carboxylic acid</td>
<td><img src="image" alt="Carboxylic acid structure" /></td>
<td>O</td>
</tr>
<tr>
<td>Ester</td>
<td><img src="image" alt="Ester structure" /></td>
<td></td>
</tr>
<tr>
<td>Thioester</td>
<td><img src="image" alt="Thioester structure" /></td>
<td></td>
</tr>
<tr>
<td>Amide (primary)</td>
<td><img src="image" alt="Amide (primary) structure" /></td>
<td>NH₂</td>
</tr>
<tr>
<td>Acid chloride</td>
<td><img src="image" alt="Acid chloride structure" /></td>
<td>Cl</td>
</tr>
<tr>
<td>Acid anhydride</td>
<td><img src="image" alt="Acid anhydride structure" /></td>
<td></td>
</tr>
</tbody>
</table>
retinol  
"the purest form of vitamin A"

acetyl salicylic acid  
(aspirin)

morphine

lysergic acid diethylamide
Alkanes

- Alkanes are "saturated" hydrocarbons - no multiple bonds
- General formula for acyclic alkanes is \( C_nH_{2n+2} \)
- The simplest example is methane

\[
\text{Angle is 109.5°} \quad \text{Bond length is 109 pm}
\]

- All C-H bond lengths (109 pm) are the same
- All \( \angle \text{H-C-H} \) angles (109.5°) are the same
- All C-H bond strengths are the same (412 kJ/mol)
- C-H single (\( \sigma \)) bonds formed through overlap of C \( \text{sp}^3 \) orbitals with H 1s orbitals

---

RECALL:

- Orbitals are grouped in shells of increasing size and energy
- Different shells contain different numbers and kinds of orbitals
- Each orbital can be occupied by two electrons
  - First shell contains: holds only 2 electrons
  - Second shell contains: 8 electrons
  - Third shell: 18 electrons

---
Hybridization: \(sp^3\) Orbitals and the Structure of Methane

- Carbon has 4 valence electrons \((2s^2\ 2p^2)\)
- In CH\(_4\), all C-H bonds are identical (tetrahedral)
- \(sp^3\) hybrid orbitals: the \(s\) orbital and three \(p\) orbitals combine to form four equivalent, tetrahedral hybrid orbitals \((sppp = sp^3)\)

For carbon’s outer shell:

\[
\begin{array}{c}
\text{Energy} \\
\uparrow
\end{array} \quad \begin{array}{c}
\text{hybridise} \\
\text{sppp } \text{hybrid orbitals}
\end{array} \quad \begin{array}{c}
\text{carbon bonding state outer shell} \\
\text{carbon ground state outer shell}
\end{array}
\]

Orbital diagrams:

\[
\begin{array}{c}
\begin{array}{c}
\text{Hybridization} \\
\text{Four tetrahedral sp}^3 \text{ orbitals}
\end{array} \\
\text{An sp}^3 \text{ orbital}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{2s} \\
\text{2pz} \\
\text{2py}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{= CH}_4
\end{array}
\end{array}
\]

© Thomson - Brooks Cole
Recall:

- **Lewis structures** show valence electrons of an atom as dots
  - Hydrogen has one dot, representing its 1s electron
  - Carbon has four dots (2s\(^2\) 2p\(^2\))

- Stable molecule → completed shell, octet (eight dots) for main-group atoms (two for hydrogen)
Hybridization: \( sp^3 \) Orbitals and the Structure of Ethane

- Two C's bond to each other by \( \sigma \) overlap of an \( sp^3 \) orbital from each
- Three \( sp^3 \) orbitals on each C overlap with H 1s orbitals to form six C-H bonds
- C-H bond strength in ethane 420 kJ/mol
- C-C bond is 154 pm long and strength is 376 kJ/mol
- All bond angles of ethane are tetrahedral
Nomenclature

How do you name an organic compound?

- Need a unique name for every unique compound
- Use IUPAC naming system
- The name has several parts:

Locates the substituent(s) in the molecule

The number of carbons in the longest chain containing the functional group

Number(s) Substituent(s) Stem Ending

The parts of the molecule that are not the stem

The functional group present

Rules

1) Find and name the longest carbon chain containing the functional group - this is the stem - and add the ending
2) Identify substituent(s)
3) Number the longest chain to give the lowest possible numbering for substituent(s)
4) Allocate a number to every substituent
5) List substituents in alphabetical order
6) Identical substituents are indicated by prefixes: di (2), tri (3), tetra (4), then penta (5), hexa (6)...then write it all out as one word
Naming Alkanes: Stems and Substituents

- Alkanes have the ending -ane
- The stem is given by the number of carbons

<table>
<thead>
<tr>
<th>Alkane</th>
<th>Alkyl substituent</th>
</tr>
</thead>
<tbody>
<tr>
<td>propane</td>
<td>CH₃CH₂CH₃</td>
</tr>
<tr>
<td>pentane</td>
<td>CH₃CH₂CH₂CH₂CH₃</td>
</tr>
</tbody>
</table>
Constitutional Isomers

· Alkanes form a homologous series of saturated hydrocarbons that differ by a CH₂ group. They have the general formula CᵣH₂ᵣ₊₂

· Molecules with the same molecular formula but a different bond connectivity are called constitutional isomers (sometimes structural isomers)

· As the number of carbons increases, the number of constitutional isomers increases rapidly

<table>
<thead>
<tr>
<th>n</th>
<th>CᵣH₂ᵣ₊₂</th>
<th>isomers</th>
<th>Constitutional formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CH₄</td>
<td>1</td>
<td>CH₄</td>
</tr>
<tr>
<td>2</td>
<td>C₂H₆</td>
<td>1</td>
<td>CH₃CH₃</td>
</tr>
<tr>
<td>3</td>
<td>C₃H₈</td>
<td>1</td>
<td>CH₃CH₂CH₃</td>
</tr>
<tr>
<td>4</td>
<td>C₄H₁₀</td>
<td>2</td>
<td>CH₃CH₂CH₂CH₃</td>
</tr>
<tr>
<td>5</td>
<td>C₅H₁₂</td>
<td>3</td>
<td>CH₃CH(CH₂)CH₃</td>
</tr>
<tr>
<td>6</td>
<td>C₆H₁₄</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>C₁₀H₂₂</td>
<td>75</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>C₂₀H₄₂</td>
<td>366 319</td>
<td></td>
</tr>
</tbody>
</table>

Constitutional isomers have different physical properties:

Butane
C₄H₁₀
melting point -138°C
boiling point -0.5°C

2-methylpropane
C₄H₁₀
melting point -160°C
boiling point -12°C

NOTE: Molecules containing heteroatoms may also have constitutional isomers with very different functional groups. For example: a compound with the molecular formula C₄H₈O may be a ketone, aldehyde, alkene/ether, alkene/alcohol, cyclic ether or cyclic alcohol.
Constitutional Isomers for $\text{C}_5\text{H}_{12}$:

- Alkanes are free to rotate about the carbon-carbon single bond. This gives rise to different spatial orientations of the hydrogens of one carbon relative to those of the other.
- These different structures are called conformational isomers or conformers.
- Example: ethane.

Conformational Isomers

- Conformational isomers are part of a class of isomers called stereoisomers.
- Stereoisomers possess the same constitution but differ in the arrangement of atoms in space.
Different conformers cannot usually be isolated from one another as they rapidly interconvert under normal conditions due to low energy barriers.

![Diagram showing energy levels and dihedral angles](image-url)
Cycloalkanes

· the two ends of the alkane 'meet up' to form 'rings'

· Cyclic saturated alkanes, general formula C\textsubscript{n}H\textsubscript{2n}

· Named as for the parent alkane, but add the prefix 'cyclo'

![cyclopentane](image)

1,3-dimethylcyclohexane

· When two substituents are attached to the ring at different positions stereoisomers are possible.

· Interconversion of the stereoisomers requires breaking of bonds. This does not occur at room temperature so the two forms may be separated from one another.

· These types of stereoisomers are called **configurational isomers**

cis-1,2-dimethylcyclopentane

trans-1,2-dimethylcyclopentane
Conformation of Cycloalkanes: Chair Structure of Cyclohexane

- Cycloalkanes are non-planar with "puckered" conformations which reduce strain energy: e.g. cyclohexane does not have a planar regular hexagon structure (implied by 2D-representation) which would require C-C-C bond angles of 120°.

- Cyclohexane adopts a "chair" conformation where all C-C-C bond angles are 109.5° and all hydrogens on adjacent carbons are perfectly staggered.

- Hydrogens occupy two positions - axial and equatorial - which are interconverted by ring "flipping" (rapid at room temperature).

\[ \text{H}_a \text{ indicates } \text{axial hydrogens} \]

\[ \text{H}_e \text{ indicates } \text{equatorial hydrogens} \]
Substituents on the ring prefer to occupy **equatorial** positions, minimising steric repulsions.
ISOMERISM

Same *molecular formula* but different structures

Isomers
- same *molecular formula*

Constitutional Isomers
- different atom connectivities

Stereoisomers
- same atom connectivity - different arrangement in space

Conformational Isomers
- differ by rotation about a single bond

Configurational Isomers
- interconversion requires breaking bonds

Enantiomers
- non-superimposable mirror images

Diastereomers
- not mirror images