SLE155 Chemistry for the Professional Sciences

Burwood and Geelong

Class 6 Hydrocarbons

Valence bond theory

Hybridisation

Structure and bonding

Nomenclature

Hydrocarbons- Alkanes

References

Blackman A, Bottle S, Schmid G, Mocerino M and Wille U (2019a), *Chemistry*, 4th edn, John Wiley & Sons, Milton, Qld.

Blackman A, Southam D, Lawrie G, Williamson N, Thompson C and Bridgeman A (2019b), *Chemistry: core concepts*, 2nd edn, John Wiley & Sons, Milton, Qld.

Valence Bond Theory

Conventions of the orbital overlap model

Each electron in a molecule is assigned to a specific orbital.

No two electrons in a molecule have identical descriptions (Pauli).

The electrons in molecules occupy the lowest energy orbital available (Aufbau).

Only the valence orbitals are needed to describe bonding.

Valence Bond Theory

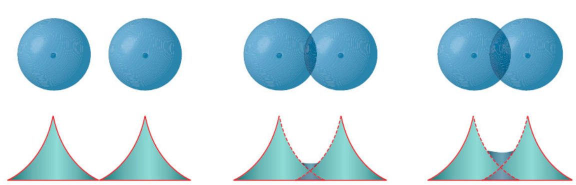
Orbital overlap

Atomic orbitals combine to form bonding orbitals.

Consider the hydrogen molecule, H_2.

As 2 hydrogen atoms approach each other, the overlap of their 1*s* orbitals increases.

Source: Blackman et al. (2019:343).



Valence bond theory

Hybridisation of atomic orbitals

- Hybrid orbitals are combinations of atomic orbitals.
- The process by which we combine them is called hybridisation.

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Valence bond theory

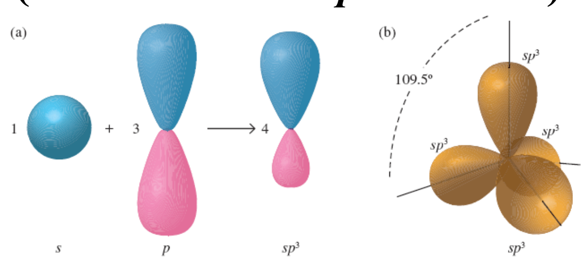
*sp*³ hybrid orbitals in methane

Electron configuration of carbon $1s^2 2s^2 2p^2$

Valence orbitals are $2s$ and $2p$ orbitals

They are mixed to form a new hybrid orbital sp^3 (¼s character – ¾p character)

Source: Blackman et al. (2019:345).



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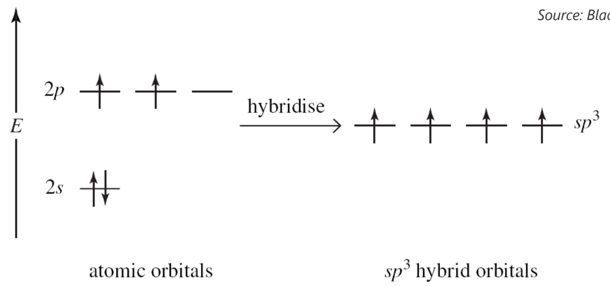
Valence bond theory

sp^3 hybrid orbitals in methane

In terms of energy energy of sp^3 hybrid orbital must be ¼ E_{2s} + ¾ E_{2p}

Source: Blackman et al. (2019:345).

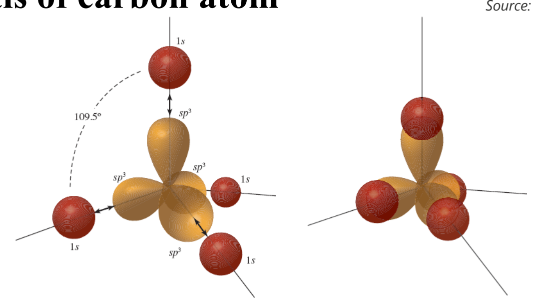


Valence bond theory

sp^3 hybrid orbitals in methane

Methane forms from orbital overlap between the hydrogen 1*s* orbitals and each of the sp^3 hybrid orbitals of carbon atom

Source: Blackman et al. (2019:346).



sp^3 hybridisation is not limited to carbon

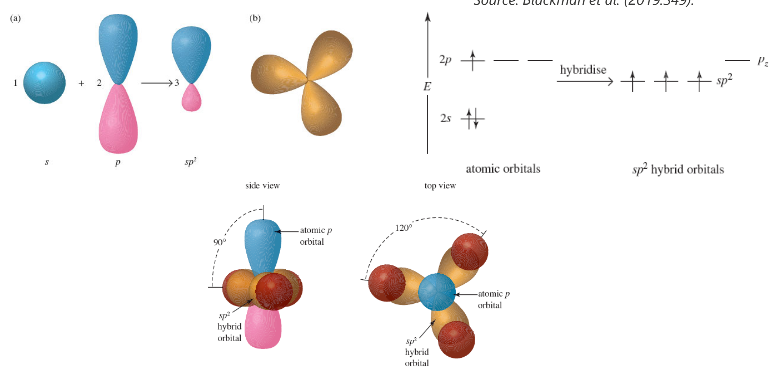
Valence bond theory

sp^2 hybrid orbitals in boron trifluoride, BF_3

Electron configuration of boron $1s^2 2s^2 2p^1$

(1/3 *s* character – 2/3 *p* character)

Source: Blackman et al. (2019:349).



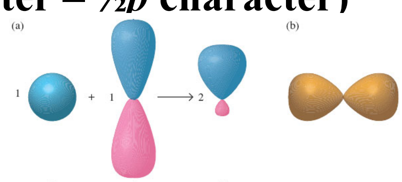
Valence bond theory

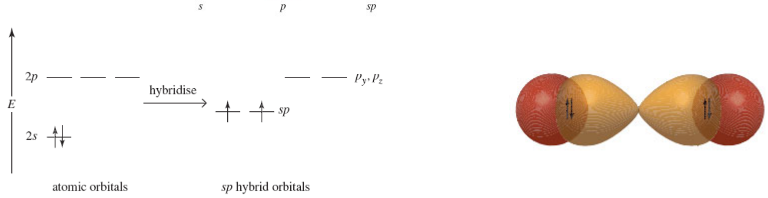
sp hybrid orbitals in beryllium dihydride, BeH_2

Electron configuration of beryllium $1s^2 2s^2$

(½*s* character – ½*p* character)

Source: Blackman et al. (2019:350).





Valence bond theory

Multiple bonds

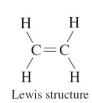
Procedure:

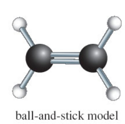
- Determine the Lewis structure
- Use the Lewis structure to determine the type of hybridisation of an atom
- Construct the σ bond framework
- Add the π bonds

Valence bond theory

Multiple bonds – ethene

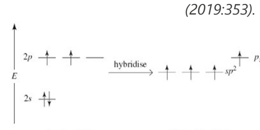
Double bond



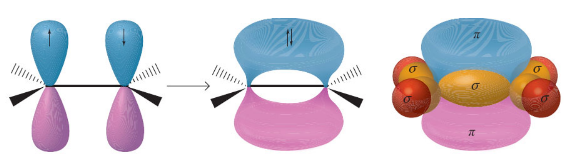


Source: Blackman et al. (2019:353).

Each carbon atom is *sp*^{2} hybridised



Orbital picture of bonding



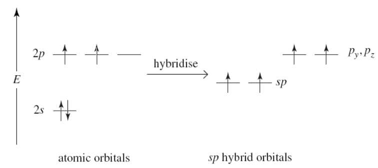
one σ bond and one π bond

Valence bond theory

Multiple bonds – ethyne

Triple bond $H-C\equiv C-H$

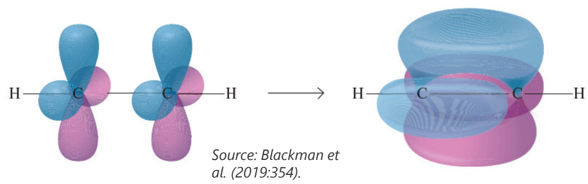
Each carbon atom is *sp* hybridised



Orbital picture of bonding

one σ bond

and two π bonds

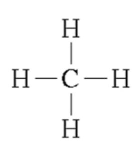


Source: Blackman et al. (2019:354).

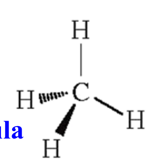
Representations of molecules

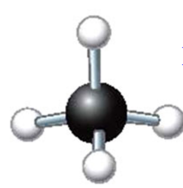
Chemical formula CH_4

Structural formula



3D structural formula





Ball and stick model

Space-filling model

Chemical formulae

The relative number of each type of atom present in a substance is shown.

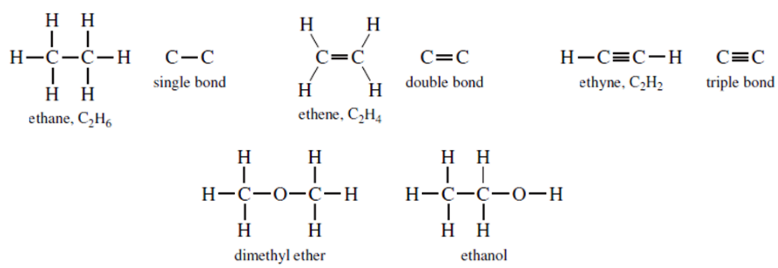
Molecular formula

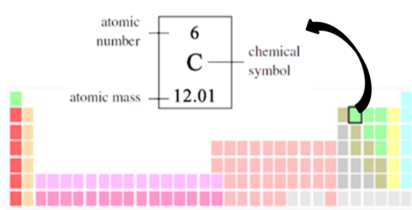
Chemical formula that refers to a discrete molecule.

Covalent compounds

Carbon first, followed by hydrogen and then the remaining elements in alphabetical order, e.g., C_2H_6O, C_4H_9BrO

Structural formulae





Catenation

Tetravalency

Structural Formulae

Carbon is a tetravalent element — this means it forms a <u>total</u> of 4 bonds when bonded to other atoms in a molecule.

These bonds may be single, double or triple bonds.

Structural formulae are useful in organic chemistry.

Representations of molecules

There are two types of shorthand structural formulae:

1. **condensed structural formulae**
2. **line structures**

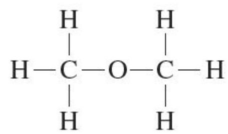
Condensed structural formulae

The constituent atoms are arranged in bonded groups, the actual bonds are not drawn.

dimethyl ether	CH_3OCH_3
ethanol	CH_3CH_2OH

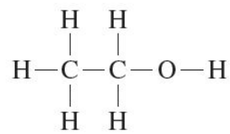
Structural Formulae

Structural formulae are essential to distinguish between isomers.



dimethyl ether

C_2H_6O



ethanol

C_2H_6O

Isomers are molecules with the same chemical formula but different structural formula.

Representations of molecules

Line structures

Use the following guidelines:

All bonds except C-H bonds are shown as lines.

Each line represents two electrons being shared.

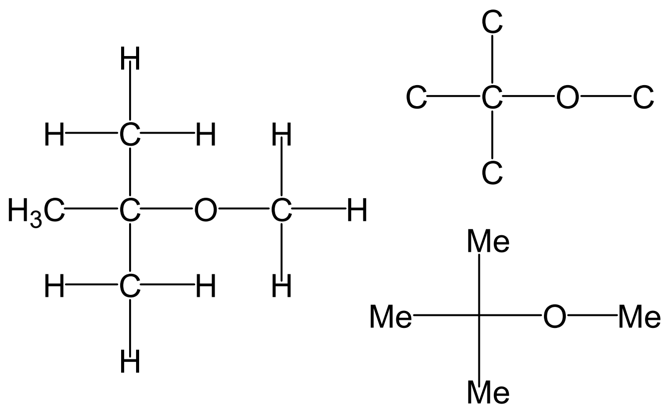
C-H bonds and H atoms attached to carbon are not shown in the line structure.

Single bonds are shown as 1 line; double bonds are shown as 2 lines; triple bonds are shown as 3 lines.

Carbon atoms are not labelled.

All other atoms are labelled with their elemental symbols.

Drawing Line Structures

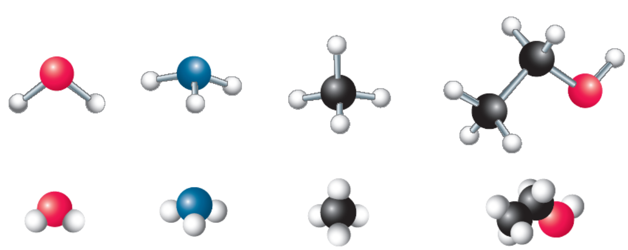


Representations of molecules

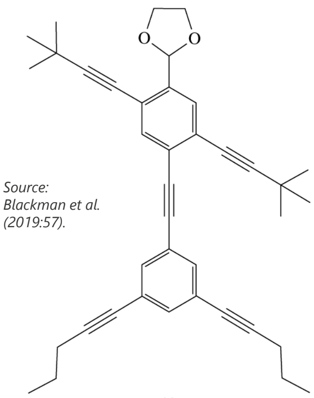
Molecule	water	ammonia	methane	ethanol
Chemical formula	H_2O	NH_3	CH_4	C_2H_6O
Structural formula	H—O—H	H—N(H)—H	CH_4: H—C(H)(H)—H	H—C(H)(H)—C(H)(H)—O—H

Ball-and-stick model

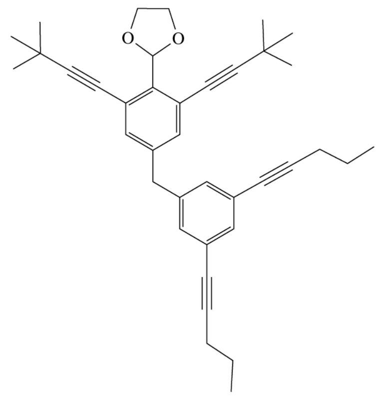
Space-filling model



Line Structures



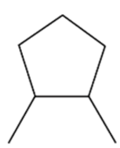
(a)



(b)

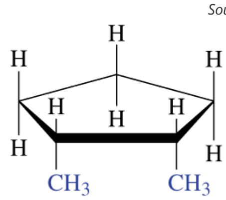
Source: Blackman et al. (2019:57).

3D Structures

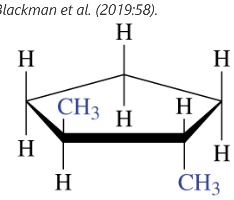


1,2-dimethylcyclopentane exists as two isomers

Source: Blackman et al. (2019:58).

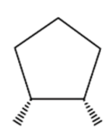


cis isomer

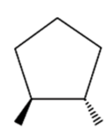


trans isomer

Represented as



cis isomer



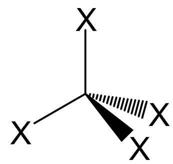
trans isomer

3D Structures

Lines represent bonds in the plane of the page.

Dotted lines or dashed wedges represent bonds going behind the plane of the page.

Solid wedges are bonds coming out of the plane of the page.

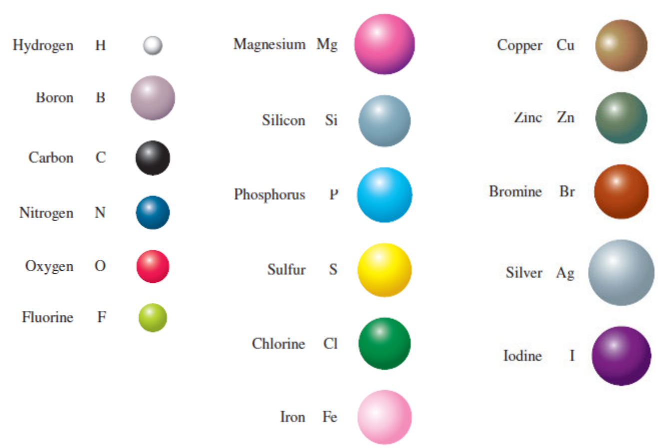


CX_4

Tetrahedral

4 bonds around a single carbon atom

3D Structures



Source: Blackman et al. (2019:59).

You will use molecular models in practical exercise 5

3D Structures

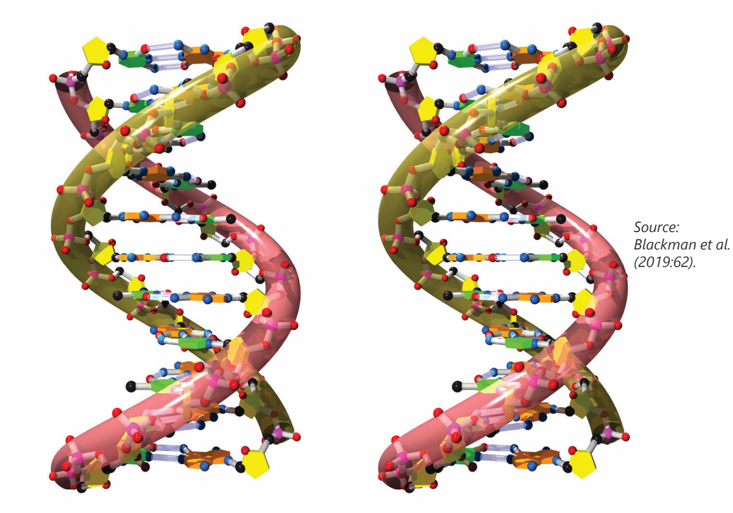


Figure 2.18 Page 49 Representation of deoxyribonucleic acid (DNA) double helix

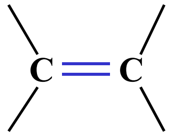
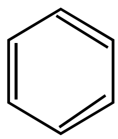
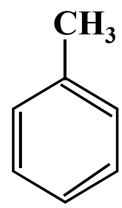
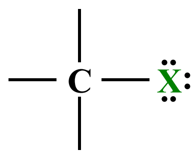
Functional Groups

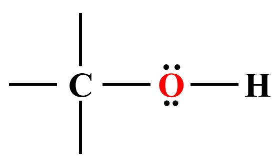
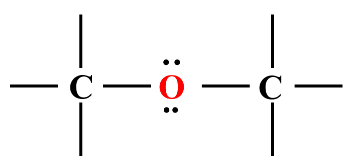
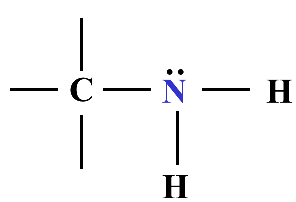
Organic compounds are composed mainly of carbon and hydrogen.

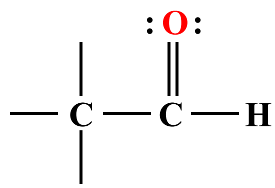
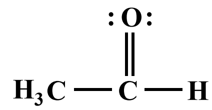
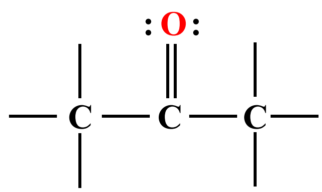
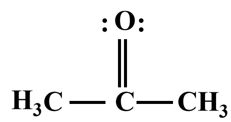
Functional groups are a characteristic feature of organic molecules that behave in a predictable way.

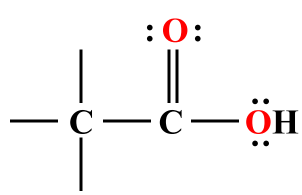
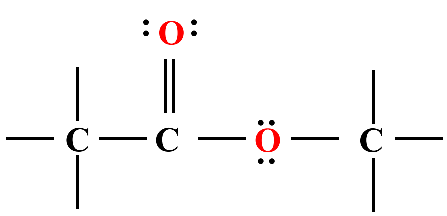
They are an atom or group of atoms that give the molecule its chemical properties.

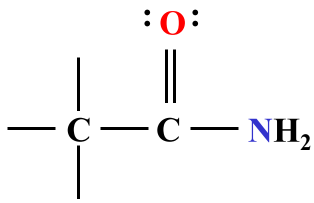
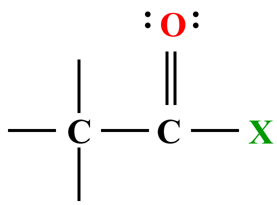
They are a way to classify families of organic compounds.

Class	Functional group	Example
alkene		$CH_3CH{=}CH_2$
alkyne	$-C{\equiv}C-$	$H-C{\equiv}C-H$
aromatic		
alkyl halide (haloalkane)		X = F, Cl, Br, I

Class	Functional group	Example
alcohol		C_2H_5OH
ether		$H_3C\text{-}O\text{-}CH_3$
amine		CH_3NH_2

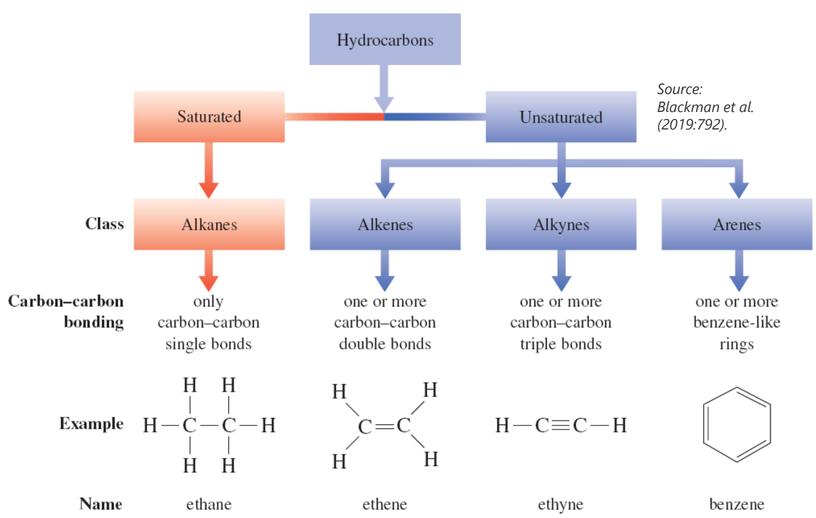
Class	Functional group	Example
aldehyde		
ketone		

Class	Functional group	Example
carboxylic acid		CH_3COOH
ester		CH_3COOCH_3

Class	Functional group	Example
amide		CH_3CONH_2
acid halide		CH_3COCl

X is F, Cl, Br or I

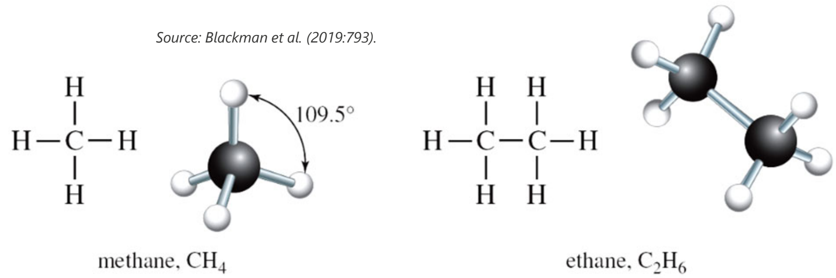
The Hydrocarbons



Alkanes

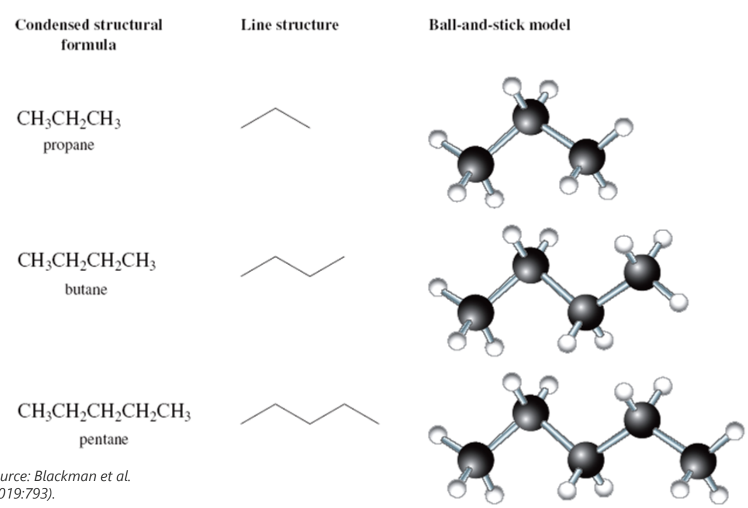
Single bonds between carbon atoms

Source: Blackman et al. (2019:793).



mean that all carbon atoms are tetrahedral with all bond angles approximately 109.5°

Alkanes



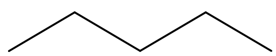
Source: Blackman et al. (2019:793).

Alkanes: Nomenclature

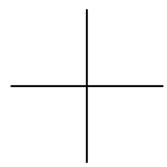
Constitutional isomerism in alkanes

These compounds have the same chemical formula but their atoms are bonded in a different order.

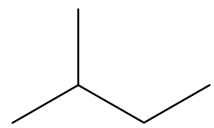
They can usually be distinguished by their different physical properties, such as melting or boiling point.



pentane



2,2-dimethylpropane

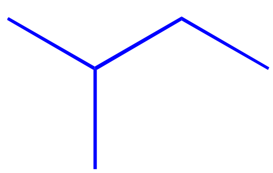


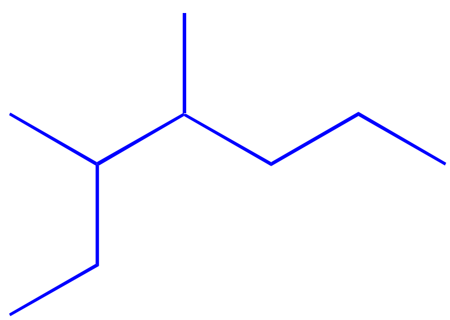
2-methylbutane

Organic Chemistry

Representation of Organic Structures

- **Chains formed by carbon atoms may be branched:**

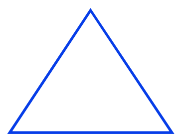




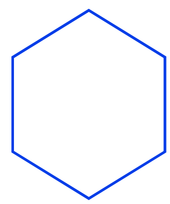
Organic Chemistry

Representation of Organic Structures

- **Compounds containing rings of carbon atoms are also common:**



cyclopropane



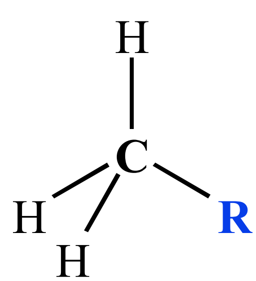
cyclohexane

Classification of C and H atoms

- **The terms primary, secondary, tertiary and quaternary are used in organic chemistry to describe carbon atoms.**

A primary (1°) C atom has one other C atom bonded to it.

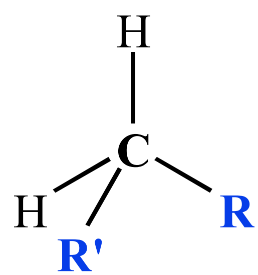
R means the rest of the molecule.



Classification of C and H atoms

- **The terms primary, secondary, tertiary and quaternary are used in organic chemistry to describe carbon atoms.**

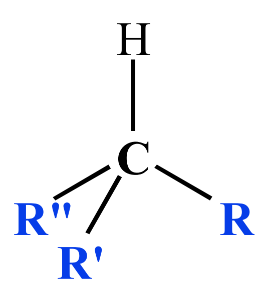
A secondary (2°) C atom has two other C atoms bonded to it.



Classification of C and H atoms

- **The terms primary, secondary, tertiary and quaternary are used in organic chemistry to describe carbon atoms.**

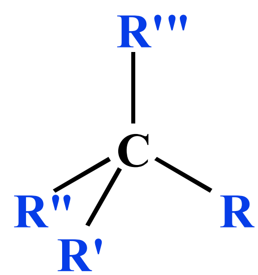
A tertiary (3°) C atom has three other C atoms bonded to it.



Classification of C and H atoms

- The terms primary, secondary, tertiary and quaternary are used in organic chemistry to describe carbon atoms.

A quaternary (4°) C atom has four other C atoms bonded to it.



Alkanes

IUPAC nomenclature

The names of all alkanes end in –*ane*

e.g., meth*ane* (CH_4), eth*ane* (C_2H_6)

The general molecular formula for alkanes is

C_nH_{2n+2}

Nomenclature: Alkanes

Molecules containing only carbon and hydrogen atoms joined by single bonds are alkanes.

They are referred to as saturated hydrocarbons.

You <u>must</u> learn these!

Prefix	Number of carbon atoms
meth-	1
eth-	2
prop-	3
but-	4
pent-	5
hex-	6
hept-	7
oct-	8
non-	9
dec-	10

DEAKIN COLLEGE

Nomenclature: Organic Compounds

Prefix:

shows the number of carbons in the parent chain

Infix:

shows the nature of the carbon bonding in the parent chain

Suffix:

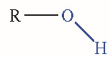
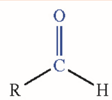
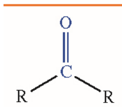
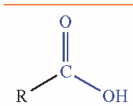
shows the functional group(s) present in the compound

Infix	Nature of carbon–carbon bonds in the parent chain
-an-	all single bonds
-en-	one or more double bonds
-yn-	one or more triple bonds

Suffix	Class of compound
-e	hydrocarbon
-ol	alcohol
-al	aldehyde
-one	ketone
-oic acid	carboxylic acid

DEAKIN COLLEGE

Nomenclature: Organic Compounds

Functional group	Name of group	Found in	R =
	hydroxyl	alcohols	C
	carbonyl	aldehydes	C or H
	carbonyl	ketones	C
	carboxyl	carboxylic acids	C or H

Some common functional groups,
Names are based on the parent molecule.

Organic Chemistry

Naming Organic Compounds

1 **Find the longest carbon chain in the molecule and use the name of that chain as the parent name.**

Organic Chemistry

Naming Organic Compounds

2 Number the carbon atoms in the longest chain beginning at the end nearest the first branch point.

This will enable the lowest combination of numbers to be used.

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Organic Chemistry

Naming Organic Compounds

3 Identify and number the substituents according to their point of attachment to the main chain.

If there are two substituents on the same carbon, assign them both the same number.

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Organic Chemistry

Naming Organic Compounds

4 **Write the name as a single word, using hyphens to separate the different prefixes and using commas to separate numbers.**

If two or more different substituents are present, name them in alphabetical order.

Organic Chemistry

Naming Organic Compounds

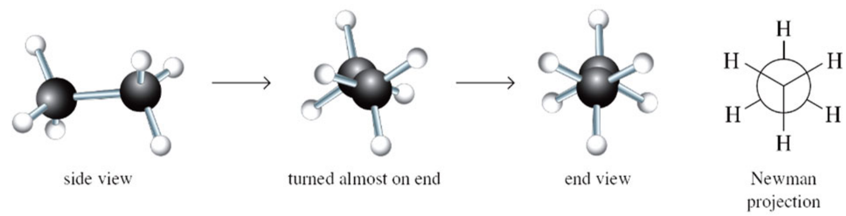
If two or more identical substituents are present, use the prefixes *di-*, *tri-*, *tetra-* to indicate how many.

Alkanes

Free rotation about carbon-carbon single bonds leads to an infinite number of conformations

Staggered conformation is most stable (lowest energy) e.g., ethane

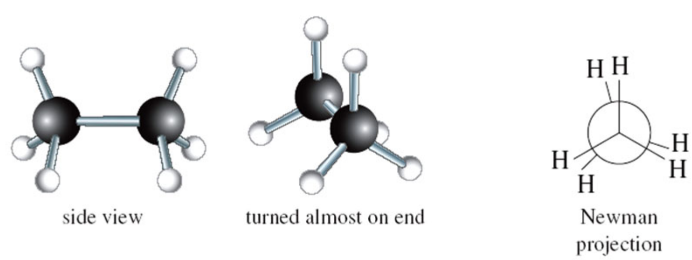
Source: Blackman et al. (2019:796).



Alkanes

Eclipsed conformation is least stable (highest energy) e.g., ethane

Source: Blackman et al. (2019:796).



Alkanes

Physical properties of alkanes

Alkanes are nonpolar compounds with weak interactions (dispersion forces) between molecules.

Boiling points will increase with size of molecule.

- alkanes with 1–4 C atoms are gases
- alkanes with 5–17 C atoms are liquids
- alkanes with >18 C atoms are waxy solids

Alkanes

Physical properties of alkanes

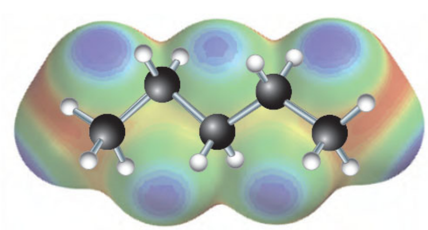
melting point and density

average density 0.7 g/mL (1–10 carbons)

isomeric alkanes

different physical properties, e.g.,

branched chain isomers will have lower boiling points than their straight chain counterparts.



Alkanes: Formulae and Naming

Name	Molecular formula	Condensed structural formula	Melting point (°C)	Boiling point (°C)	Density of liquid (g mL^{-1} at 0 °C)[a]
methane	CH_4	CH_4	–182	–164	(a gas)
ethane	C_2H_6	CH_3CH_3	–183	–88	(a gas)
propane	C_3H_8	$CH_3CH_2CH_3$	–190	–42	(a gas)
butane	C_4H_{10}	$CH_3(CH_2)_2CH_3$	–138	0	(a gas)
pentane	C_5H_{12}	$CH_3(CH_2)_3CH_3$	–130	36	0.626
hexane	C_6H_{14}	$CH_3(CH_2)_4CH_3$	–95	69	0.659
heptane	C_7H_{16}	$CH_3(CH_2)_5CH_3$	–90	98	0.684
octane	C_8H_{18}	$CH_3(CH_2)_6CH_3$	–57	126	0.703
nonane	C_9H_{20}	$CH_3(CH_2)_7CH_3$	–51	151	0.718
decane	$C_{10}H_{22}$	$CH_3(CH_2)_8CH_3$	–30	174	0.730

(a) For comparison, the density of H_2O is 1 g mL^{-1} at 4 °C.

Source: Blackman et al. (2019:794).

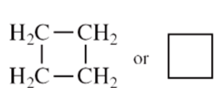
Alkanes

Cycloalkanes

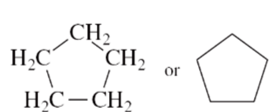
carbon-carbon single bonds in a ring

five-membered and six-membered rings are the most common

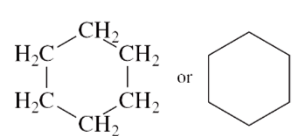
general formula: C_nH_{2n}



cyclobutane



cyclopentane

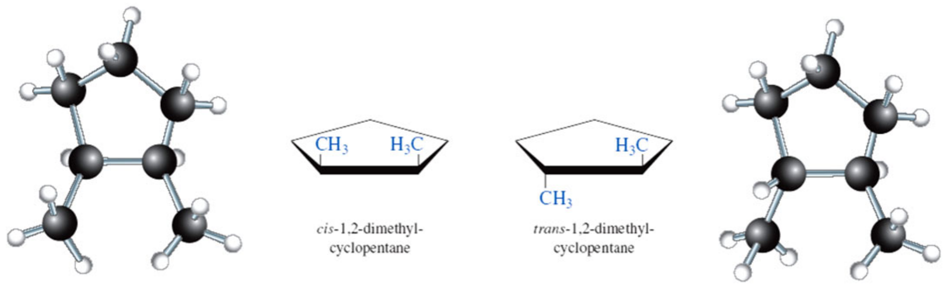


cyclohexane

Alkanes

***cis-trans* isomerism in cycloalkanes**

arrangement of atoms in space that cannot be changed by rotation around sigma bonds

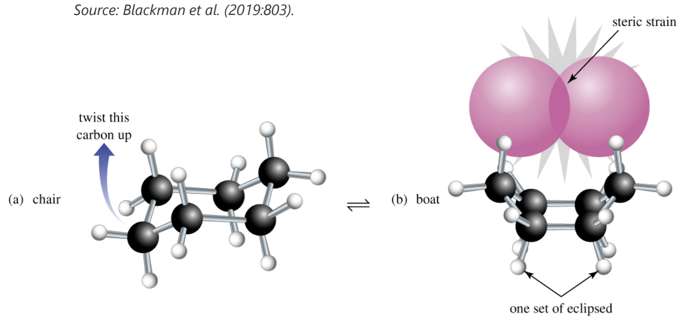


Saturated Hydrocarbons

Cycloalkanes

- **Cyclohexane occurs widely in nature**
- **The most stable conformation is the chair conformation with all bond angles 109.5°.**

Source: Blackman et al. (2019:803).



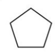
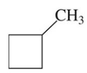
Boiling Points of Pentanes

Boiling points of alkanes are low, but increase with larger molecules due to increased dispersion forces.

Branched alkanes have lower boiling points than their straight chain isomers.

Cycloalkanes with the same number of C atoms have higher boiling points than their open chain counterparts.

Comparison of Boiling Points of Alkanes and Cycloalkanes with Five Carbons

Formula	Name	Boiling Point (°C)
Cycloalkanes		
	cyclopentane	49
	methylcyclobutane	36.3
Continuous alkane		
$CH_3—CH_2—CH_2—CH_2—CH_3$	pentane	36
Branched alkanes		
$CH_3—CH(CH_3)—CH_2—CH_3$	2-methylbutane	28
$CH_3—C(CH_3)_2—CH_3$	dimethylpropane	10