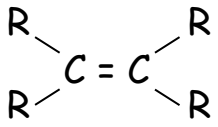
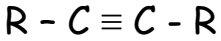
2.1a Molecular Orbitals

Functional Groups

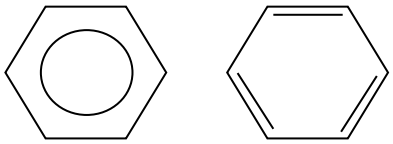
a) Groups Containing Carbon and Hydrogen Only



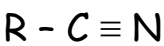
alkene



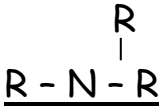
alkyne


aromatic

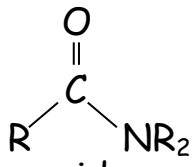
b) Functional Groups Containing Nitrogen



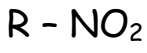
nitrile



amine

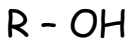


amide

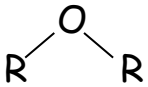


nitro-

c) Functional Groups Containing Oxygen and Single Bonds

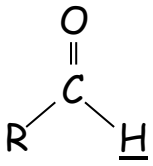


alcohol

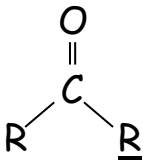


ether

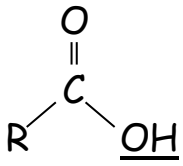
d) Functional Groups Containing Oxygen and Double Bonds



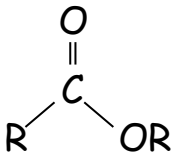
aldehyde



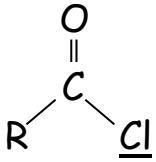
ketone



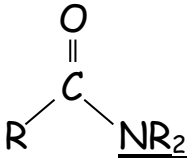
carboxylic acid



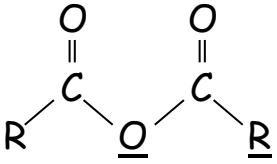
ester



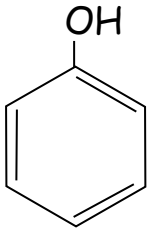
acid chloride



amide

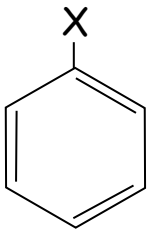


acid anhydride



phenol

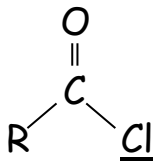
e) Functional Groups Containing Halogens



aryl halide

R – X

alkyl halide

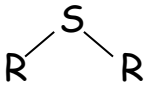


acid chloride

f) Functional Groups Containing Sulphur

R – SH

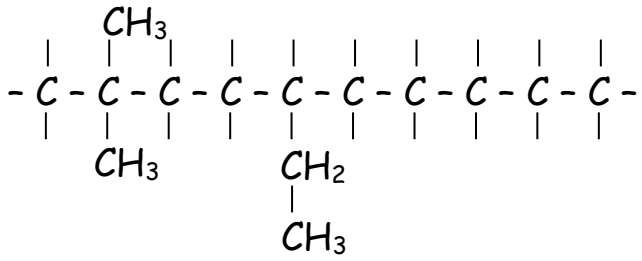
thiol



thioether

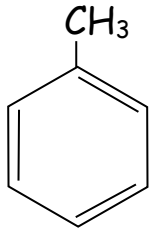
Revision of Nomenclature

a) Sidegroups listed alphabetically (ignoring mono-, di-, tri-, etc)

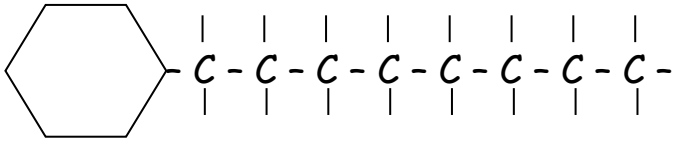


5-ethyl-2,2-dimethyldecane

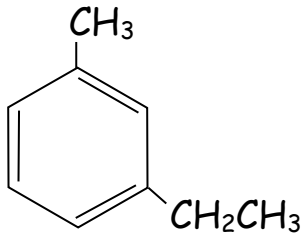
b) Which functional group has priority



methylbenzene



1-cyclohexyloctane



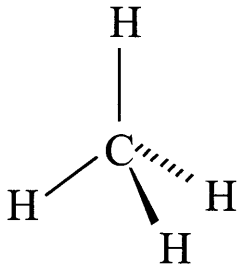
1-ethyl-3-methylbenzene

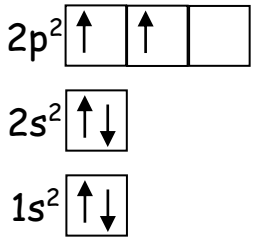
Bonding in Alkanes

Free atoms of carbon have the electron arrangement of $1s^2$, $2s^2$, $2p^2$.

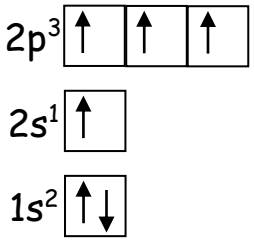
- 2 unpaired electrons in the 2p suborbital
- Expected valency of carbon would be 2 from this information

However, we know carbon has a valency of 4 and carbon forms 4 C-H bonds in methane.

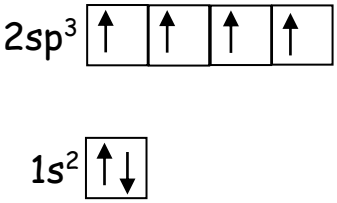




Isolated carbon atom



Carbon atom with promoted electron

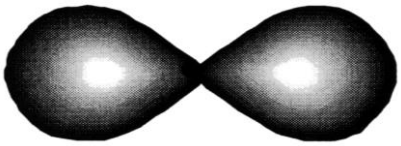


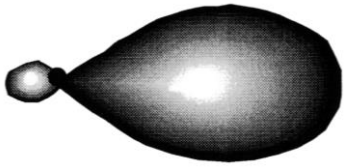
Carbon atom after hybridisation

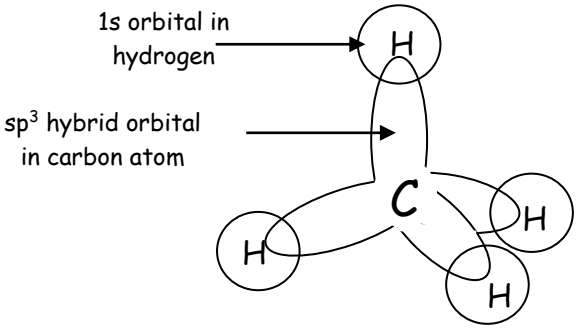
- Mixing of atomic s and p orbitals to generate a new set of hybrid orbitals

- Energy required to promote electron is overcome by
  - better shape for forming bonds
  - the energy released when forming new bonds

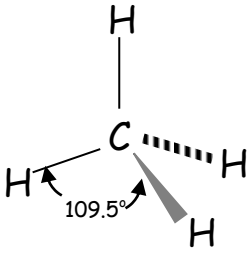
Sigma Bonds & sp_3 Hybridisation

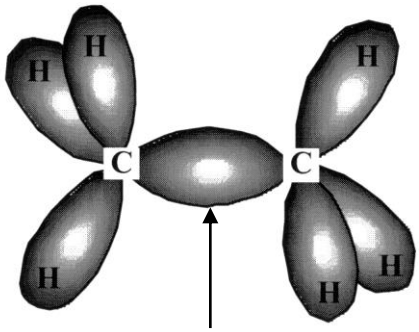
- p-orbitals have the shape 

- one sp^3 hybrid orbital has the shape 



methane CH_4





ethane C_2H_6

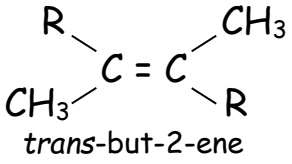
Sigma (σ) bond

End-on overlap of atomic orbitals lying along the axis of the covalent bond

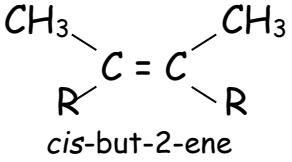
- sigma (single) bonds are rotatory
  - allows rotation around the axis of the sigma bond

Bonding in Alkenes (Π-bonds)

- Alkenes contain C=C double bond
- Bond angle in ethene is 120°
- Ethene is a planar molecule
- C=C double bond is shorter in length than the C-C single bond
- Double bonds do not rotate around the axis of the C=C double bond
    - *trans*- and *cis*- geometric isomers exist since C=C double bond does not rotate (see Unit 2.2 Stereochemistry)



trans-but-2-ene

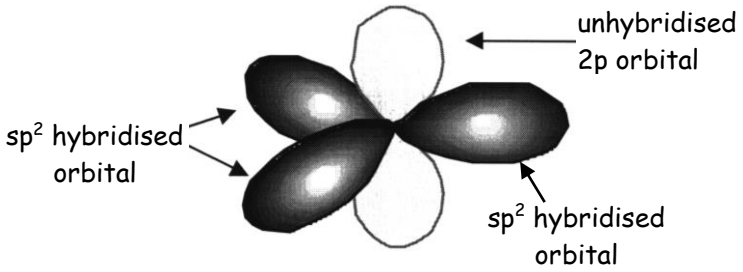


cis-but-2-ene

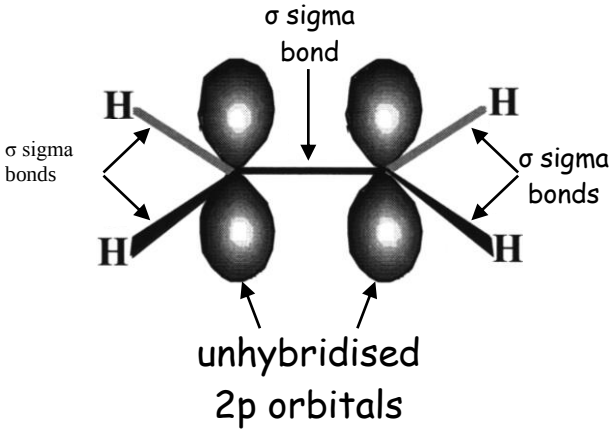
Bond	C–C	C=C	C≡C
Bond Enthalpy (kJ mol^{-1})	337	607	828
Bond Length (nm)	0.154	0.134	0.121

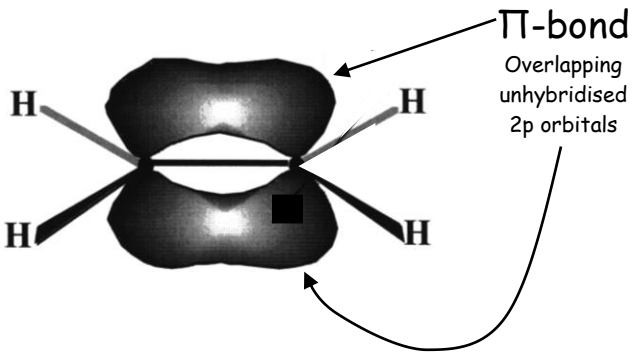
sp^2 Hybridisation

- alkenes hybridise their orbitals differently to alkanes



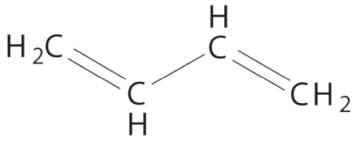
- ethene has the following bonding arrangement
    - central bond formed by overlap of sp^2 hybridised orbitals
    - 2nd bond formed by the overlap of the 2 unhybridised 2p orbitals
    - Π-bond has high electron density located in 2 areas on either side of the σ–bond
    - Π–bond in C=C double bond is shorter and weaker than the σ–bond in C-C in alkanes (see above table)



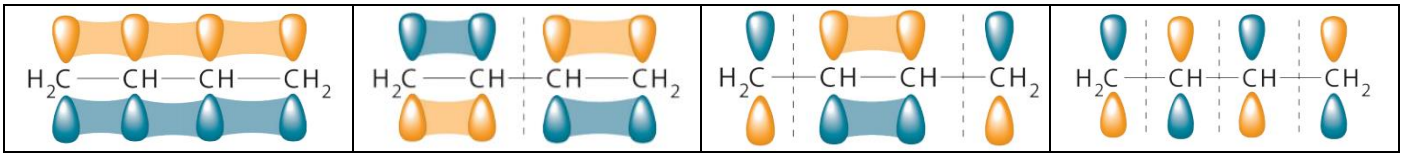


Colour in Organic Molecules - Conjugated Systems

A conjugated system exists when a molecule has alternating single and double bonds.
For example, buta-1,3-diene has the structure:



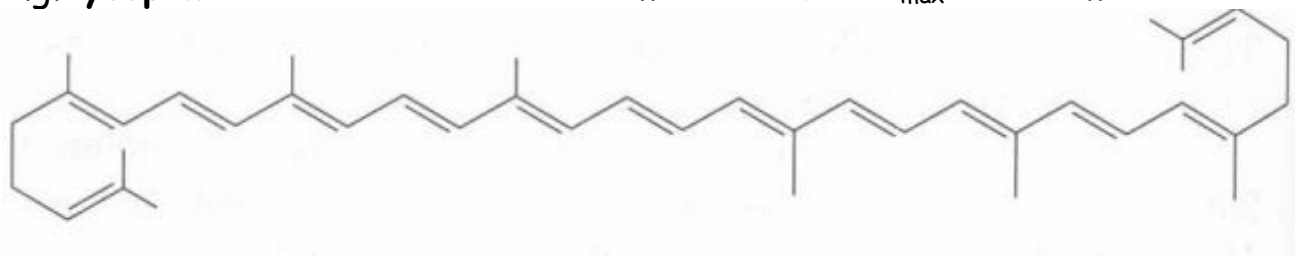
Each carbon has sp^2 hybridisation forming 3 sigma bonds on each carbon. This leaves four unhybridised p-orbitals over the four carbons to overlap to form two pi bonds. There are four options:



Most stable ◄——————————————► Least stable
(lower energy) (higher energy)

Buta-1,3-diene absorbs only in the UV region of the electromagnetic spectrum but molecules with larger conjugated systems will absorb from the Visible spectrum and produce colours.

e.g. **lycopene** causes red colour in tomatoes where λ_{max} = 505nm



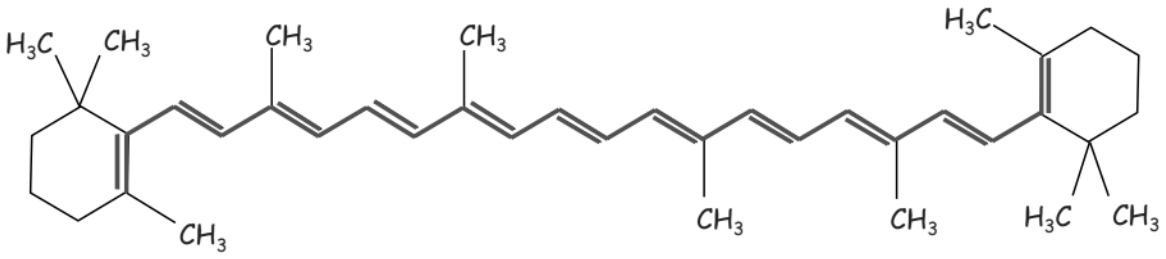
The section of a molecule with alternating double and single bonds in the carbon chain is called a conjugated system. Electrons are delocalised, within molecular orbitals, across the conjugated system

- The more atoms in a conjugated system the smaller the energy gap between the higher occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO)
- The smaller the energy gap the lower the energy of the light absorbed
    - Lower energy of light = lower frequency = higher wavelength.
- The non-absorbed wavelengths of visible light are then transmitted and the complimentary colour is seen

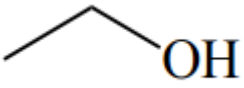
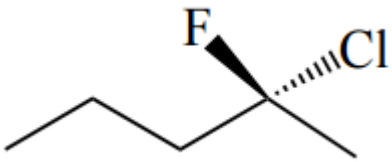
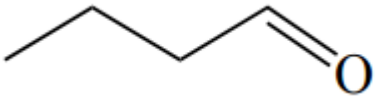
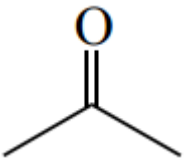
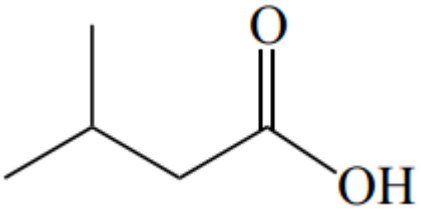
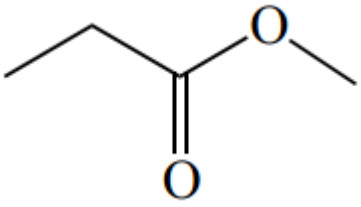
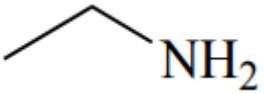
Most organic molecules appear colourless because the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) is relatively large and the energy is in the ultraviolet region of the EM spectrum.

Chromophores is a group of atoms within an organic molecule which is responsible for the absorption of light in the visible region of the EM spectrum.

- If light is absorbed of one colour then the compound will exhibit the complimentary colour of the transmitted (non-absorbed) wavelengths
- Light is absorbed when electrons in the chromophore are promoted from the HOMO to the LUMO.



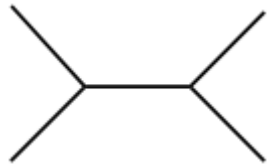
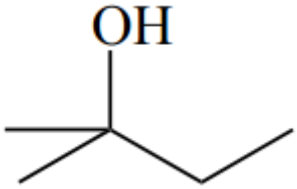
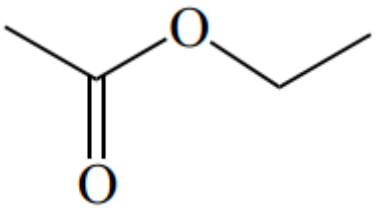
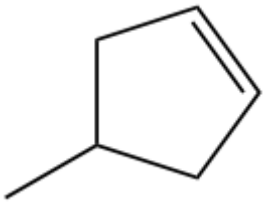
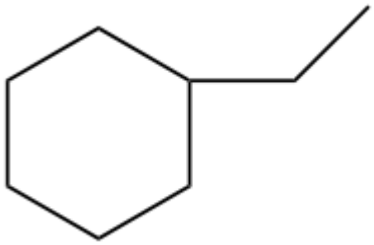
2.1b Molecular Structure

	Name	Skeletal Structure
a)	hexane	
b)	hex-3-ene	
c)	ethanol	
d)	2-chloro-2-fluoropentane	
e)	butanal	
f)	propanone	
g)	3-methylbutanoic acid	
h)	methylpropanoate	
i)	1-aminoethane or ethylamine	

Draw skeletal diagrams for each of the following:

a)	Propane	$CH_3CH_2CH_3$	
b)	Methoxymethane	CH_3OCH_3	
c)	Propyne	$HC{\equiv}CCH_3$	
d)	Ethanal	CH_3CHO	
e)	Tetrafluoroethene	$F_2C{=}CF_2$	
f)	Propadiene	$CH_2{=}C{=}CH_2$	

Name and draw the full structural formula of the following skeletal structures

	Skeletal Structure	Full Structural Formula	Name
a)			
b)			
c)			
d)			
e)			

Also 2016 AH Chem L7b(iii) and 2015 revAH Chem MC11